# COMPUTATIONAL MODELING AND OPTIMIZATION OF A MULTIPLE TUBE AEROSOL FLOW REACTOR FOR HIGH TEMPERATURE SOLAR-THERMAL PROCESSES

by

# JANNA GAIL MARTINEK B.S., University of Colorado-Boulder, 2005

A thesis submitted to the Faculty of the Graduate School of the University of Colorado in partial fulfillment of the requirement for the degree of Doctor of Philosophy Department of Chemical and Biological Engineering 2012 This thesis entitled:

Computational Modeling and Optimization of a Multiple Tube Aerosol Flow Reactor for High Temperature Solar-Thermal Processes

written by Janna Gail Martinek

has been approved for the Department of Chemical and Biological Engineering

Alan W. Weimer (Chair)

Christine Hrenya

Date\_\_\_\_\_

The final copy of this thesis has been examined by the signatories, and we find that both the content and the form meet acceptable presentation standards of scholarly work in the above mentioned discipline.

Martinek, Janna Gail (Ph.D., Chemical and Biological Engineering)

Computational Modeling and Optimization of a Multiple Tube Aerosol Flow Reactor for High

Temperature Solar-Thermal Processes

Thesis directed by Professor Alan W. Weimer

Concentrated solar energy can be used to provide the heat necessary to drive highly endothermic chemical reactions for renewable fuel production including thermal reduction of metal oxides for water-splitting cycles, and gasification of cellulosic biomass. A computational model coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics is developed for a solar receiver comprised of a specularly reflective cylindrical cavity with a windowed aperture and an array of five tubes. Finite volume techniques for radiative transfer provide accurate depictions of diffuse energy emitted by heated surfaces, but fail to produce viable solutions for solar energy with computationally reasonable mesh sizes. A hybrid Monte Carlo/finite volume strategy is proposed for radiative transfer and coupled with a three-dimensional steady state computational fluid dynamics model describing steam gasification of acetylene black. Maximum predicted temperatures for 6 kW solar power are 1813 K, 1343 K, and 1546 K at the center, front, and back tubes respectively, with corresponding reaction conversions of 40%, 2.5%, and 9.2%. Average discrepancies between temperatures predicted via the computational model and those experimentally measured on-sun up to 1700 K are 21-44 K (2-4%) for both ceramic and metallic tube materials. Predicted solar-to-chemical receiver efficiency is less than 4% with conduction and emission losses accounting for 55-69% and 11-25% of the solar input, respectively.

Parameters describing operating conditions and receiver geometry are exploited to optimize the solar-to-chemical efficiency for both cooled reflective and insulated absorbing cavity designs scaled to accept 8 kW solar power. Tubes positioned outside of the solar beam fail to achieve adequate reaction conversion and contribute heavily to conduction losses in reflective cavity designs. Ideal configurations produce up to 13% solar-to-chemical efficiency and contain three moderately sized tubes situated within the solar beam and set back from the aperture such that a portion of the solar energy reflects off of the cavity wall. Insulated absorbing cavity designs are characterized by comparatively greater temperature uniformity, higher reaction conversion, and diminished conduction losses. Ideal configurations produce up to 35% efficiency and contain three large tubes which may be partially located outside of the solar beam.

### **CONTENTS**

### CHAPTER

I

INTRC	DUCT	ΓΙΟΝ, BACKGROUND AND SCOPE	
1.1	Motiv	ation and Scope	1
	1.1.1	Motivation	1
	1.1.2	Scope	4
1.2	Backg	ground and literature review	7
	1.2.1	Solar-thermal processes	7
	1.2.2	Design and efficiency of current receivers	10
	1.2.3	Transport and radiation modeling	13
	1.2.4	Modeling gasification kinetics	16
	1.2.5	Receiver optimization	19
Referen	nces	-	20

# II THERMODYNAMIC AND PRACTICAL LIMITATIONS ON RECEIVER EFFICIENCY

2.1	Abstract		
2.2	Introduction		
2.3	Theory		
2.4	Results		
2.5	Conclusions	41	
Nomenclature			
Refere	References		

### III DEVELOPMENT OF A MONTE CARLO MODEL FOR TRANSPORT OF SOLAR RADIATION

3.1	Introd	roduction		
3.2	Development of the model		46	
	3.2.1	Specification of wavelength	51	
	3.2.2	Specification of initial ray position	51	
	3.2.3	Specification of initial ray direction	54	
	3.2.4	Reflection/transmission at external window surface	58	
	3.2.5	Selection of surface interaction	59	
	3.2.6	Selection of surface reflection/absorption	60	
	3.2.7	Extension to emission by heated surface	64	
3.3	Comp	arison of model results with configuration factors	65	
3.4	Concl	usions	69	
Nome	nclature	e	70	
Refere	ences		72	

	EIVERTOR HIGH TEIVILERATURE SOLAR THERIVIAL F	ROCESSES _
4.1	Abstract	7
4.2	Introduction	7
4.3	Radiation models	7
	4.3.1 Finite Volume method	7
	4.3.2 Monte Carlo method	8
4.4	Results and Discussion	8
	4.4.1 Collimated incident solar radiation	8
	4.4.2 Diffuse incident solar radiation	8
	4.4.3 Solar absorption efficiency	9
	4.4.4 Emitted energy	9
	4.4.5 Evaluation of 3D finite volume models	10
4.6	Overall Modeling Strategy	10
4.7	Conclusions	10
Nom	enclature	10
Refe	rences	10

vi

V

COMPUTATIONAL MODELING AND ON-SUN MODEL VALIDATION
FOR A MULTIPLE TUBE SOLAR AEROSOL FLOW REACTOR
WITH SPECULARLY REFLECTIVE CAVITY WALLS

5.1	Abstract		
5.2	Introduction		
5.3	Radia	tion model	114
	5.3.1	Characterization of the solar flux profile	114
	5.3.2	Modeling strategy for radiation in the receiver cavity	119
	5.3.3	Monte Carlo model for solar radiation	121
	5.3.4	Finite volume model for emitted energy	126
	5.3.5	Optical properties	133
5.4	Fluid	flow models	139
	5.4.1	Dimensionless parameters and characteristic times	139
	5.4.2	Fluid flow model	141
	5.4.3	Fluid properties	144
5.5	React	ion models	146
	5.5.1	Reaction processes and equilibrium compositions	146
	5.5.2	Surface reaction mechanism for steam gasification	147
	5.5.3	Particle reaction model	149
	5.5.4	Global reaction model	151
	5.5.5	Water gas shift reaction	154
5.6	Comb	ination and solution of radiation, fluid flow and	
	reaction	on models	154
	5.6.1	Boundary conditions, discretization schemes and	
		convergence criteria	156
5.7	Resul	ts and Discussion	158

5.7.1	Physical properties and model input parameters	158
5.7.2	Simulation results	161
5.7.3	Evaluation of east/west symmetry assumption	173
5.7.4	Angular and spatial mesh verification	174
5.7.5	Comparison with perfectly mixed ideal plug	
	flow solution	178
5.7.6	Comparison with water-gas shift equilibrium	
	compositions	180
Sensit	ivity analysis	181
Exper	imental Validation	186
5.9.1	Experimental Setup	186
5.9.2	Experimental validation of total solar power input	188
5.9.3	Experimental validation for temperature profiles	190
5.9.4	Experimental validation for carbon gasification	199
Concl	usions	202
nclature	2	205
nces		210
	5.7.1 5.7.2 5.7.3 5.7.4 5.7.5 5.7.6 Sensit Exper 5.9.1 5.9.2 5.9.3 5.9.4 Concl nclature	<ul> <li>5.7.1 Physical properties and model input parameters</li></ul>

### VI OPTIMIZATION STUDIES FOR A MULTIPLE TUBE SOLAR RECEIVER BASED ON COMBINED RADIATION AND COMPUTATIONAL FLUID DYNAMICS MODELING: REFLECTIVE CAVITY

6.1	Abstra		
6.2	Introd	uction	
6.3	Metho	ods	
	6.3.1	Receiver model	
	6.3.2	Specification of parameters describing receiver	
		geometry and operating conditions	
6.4	Design	n 1	
	6.4.1	Evaluation of effects	
	6.4.2	Relationship between responses	
6.5	Desig	n 2	
	6.5.1	Evaluation of effects	
	6.5.2	Effect of tube radius	
	6.5.3	Relationship between responses	
6.6	Desig	n 3	
	6.6.1	Evaluation of effects	
	6.6.2	Relationship between responses	
6.7	Desig	n 4	
6.8	Desig	n 5	
6.9	Comp	arison of original and optimal designs	
6.10	Evalu	ation of the optimal design at 1 MW	
6.11	Concl	usions	
Nome	enclature	2	
Refer	ences		

VII	OPTI	IMIZATION STUDIES FOR A MULTIPLE TUBE SOLAR	
	REC	EIVER BASED ON COMBINED RADIATION AND	
	COM	IPUTATIONAL FLUID DYNAMICS MODELING:	
	ABS	ORBING CAVITY	
	7.1	Abstract	271
	7.2	Introduction	272
	7.3	Receiver model	273
		7.3.1 Reflective vs. absorbing cavity model results	
	7.4	Design 1	
		7.4.1 Evaluation of effects	
		7.4.2 Relationship between responses	
	7.5	Design 2	
		7.5.1 Evaluation of effects	
		7.5.2 Relationship between responses	291
	7.6	Design 3	293
	7.7	Comparison between optimal and original designs	
	7.8	Evaluation of the optimal design at 1 MW	
	7.9	Conclusions	
	Nom	enclature	305
	Refe	rences	
VIII	CON	ICLUSIONS AND FUTURE DIRECTIONS	
	8.1	Summary and conclusions	
	8.2	Future research directions	
BIBLIOGRA	APHY		

# APPENDIX

A C	CHARACTERISTIC TIMES AND DIMENSIONLESS PARAMETERS A.1 Characteristic times	337
I	A.2 Dimensionless parameters	340
Ι	References	347
B C C H H	COMPARISON OF FLUID PROPERTIES PREDICTED BY CORRELATIONS WITH LITERATURE DATA 3.1 Chapman Enskog, Eucken and modified Eucken models 3.2 Comparison of model predictions with literature data References	348 349 353

С	SPEC	SPECIFICATION OF TUBE POSITIONS FOR OPTIMIZATION		
	C.1	Method A	354	
	C.2	Method B		
D	TUB	E CONFIGURATIONS, OPERATING CONDITIONS,		
	AND	RESULTS FOR OPTIMIZATION STUDIES		
	D.1	Reflective cavity	359	
	D.2	Absorbing cavity		
Е	PREI	DICTED ERRORS IN TEMPERATURE MEASUREMENTS		
	E.1	Heat transfer model		
	E.2	Comparison of temperatures measured on-sun with		
		theoretical models		
	Nom	enclature		
	Refe	rences		

# LIST OF TABLES

# Table

2.1	Calculated values of the coefficient in equation 2.4	35
3.1	Geometric surfaces and surface normal vectors describing receiver geometry	49
3.2	Monte Carlo calculations of configuration factors between a cylinder and concentric annular disk compared with analytical solutions	67
3.3	Monte Carlo calculations for configuration factors between a finite rectangle and finite cylinder of equal length compared with literature values	68
3.4	Monte Carlo calculations for configuration factors between a finite cylinder and finite rectangle of equal length compared with literature values	68
4.1	Maximum error in normalized surface heat flux and absorption efficiency	81
4.2	Approximate solution time (s) for the 2D FV method for the five tube configuration with collimated solar radiation	82
4.3	Approximate solution time (s) for the 2D MC method with 10 <sup>7</sup> rays	82
4.4	Solar absorption efficiency errors $(\eta_{abs,FV} - \eta_{abs,MC})$ for the single tube configuration	95
4.5	Solar absorption efficiency errors $(\eta_{abs,FV} - \eta_{abs,MC})$ for the five tube configuration	96
4.6	Emitted energy absorption efficiency errors $(\eta_{abs,FV} - \eta_{abs,MC})$ for the single tube configuration.	101
4.7	Emitted energy absorption efficiency errors $(\eta_{abs,FV} - \eta_{abs,MC})$ for the five tube configuration	102
5.1	Maximum and average errors in absorbed solar flux	122
5.2	Solar absorption efficiencies and reflection losses as a function of attenuator opening	125
5.3	Summary of surface optical property inputs to Monte Carlo and finite volume radiation models	133

5.4	Dimensionless parameters and characteristic times for typical operating conditions	150
5.5	Simulation input parameters: constants	159
5.6	Simulation input parameters: solid properties	159
5.7	Simulation input parameters : carbon particle properties	160
5.8	Simulation input parameters: fluid properties (300 K $< T < 2200$ K)	160
5.9	Simulation input parameters: reaction parameters	161
5.10	Simulation input parameters: operating and inlet conditions	161
5.11	Comparison of temperature, reaction conversion, and absorbed radiative energy between tubes for a 6 kW solar power input	169
5.12	Heat loss distributions as a function of incident solar power	171
5.13	Convective and conductive heat losses as a function of solar power input	172
5.14	Solar and emitted (IR) energy absorbed in individual east and west side simulations	173
5.15	Maximum errors relative to solutions on a spatial grid of 555,642 mesh elements with $(N_{\theta} x N_{\Phi}) = (9x9)$	175
5.16	Maximum errors relative to solutions on an angular grid of $(N_{\theta} x N_{\phi}) = (11x11)$ with 295,864 spatial mesh elements	175
5.17	Maximum errors relative to solutions on a center tube spatial grid of 108,486 mesh elements with $(N_{\theta} x N_{\phi}) = (5x5)$	177
5.18	Maximum errors in a simulation with $(N_{\theta} x N_{\phi}) = (5x5)$ relative to $(N_{\theta} x N_{\phi}) = (9x9)$ with a center tube spatial grid of 17,934 elements	177
5.19	Sensitivity of simulation results to 15% variability in physical and optical properties	182
5.20	Sensitivity of simulation results to 15-100% variability in particle properties	184
5.21	Approximate tube-window radiation configuration factors predicted from Monte Carlo calculations	192

xi

5.22	Comparison between experimental heat loss distributions for silicon carbide and Inconel tubes	199
5.23	Inlet boundary conditions for the carbon gasification model	
5.24	Literature values for kinetic parameters describing the steam gasification reaction	202
6.1	Factor levels for Design 1 ( $2^{13-8}$ fractional factorial): reflective cavity	
6.2	Effect magnitudes for Design 1 (2 <sup>13-8</sup> fractional factorial): reflective cavity	229
6.3	Average efficiency at treatment combinations involving $C_{feed}$ , $Q_s$ , $N_{max}$ , and $r_{cav}$	230
6.4	Geometric factor levels for Design 2 (2 <sup>6-2</sup> fractional factorial): reflective cavity	237
6.5	Effect magnitudes for Design 2 ( $2^{6-2}$ fractional factorial): reflective cavity	238
6.6	Average efficiency at various treatment combinations from Design 2	
6.7	Comparison of receiver configurations with increasing tube radius	242
6.8	Factor levels for Design 3 (2 <sup>8-4</sup> fractional factorial): reflective cavity	
6.9	Effect magnitudes for Design 3 ( $2^{8-4}$ fractional factorial): reflective cavity	249
6.10	Factor levels and main effects magnitudes for Design 4 (2 <sup>3-1</sup> fractional factorial): reflective cavity	253
6.11	Factor levels for Design 5 (five factor CCD): reflective cavity	255
6.12	Optimal design parameters and results for a reflective cavity	
6.13	Comparison of optimal and original reflective cavity receiver designs with $Q_s = 7.5$ kW and $C_{feed} = 7.6$ g/min	260
6.14	Performance of the optimal small-scale reflective cavity receiver configuration at 7.5 kW and 1 MW	
7.1	Comparison of calculations with a cooled reflective or insulated absorbing cavity wall for the existing receiver configuration	276

xii

7.2	Factor levels for Design 1 (2 <sup>13-8</sup> fractional factorial): absorbing cavity	
7.3	Effect magnitudes for Design 1 (2 <sup>13-8</sup> fractional factorial): absorbing cavity	282
7.4	Geometric factor levels for Design 2 ( $2^{6-2}$ fractional factorial): absorbing cavity	288
7.5	Effect magnitudes for Design 2 (2 <sup>6-2</sup> fractional factorial): absorbing cavity	288
7.6	Average efficiency at various treatment combinations from Design 2	290
7.7	Factor levels for Design 3 (five factor CCD): absorbing cavity	295
7.8	Optimal design parameters and results for an absorbing cavity	296
7.9	Comparison of optimal and original absorbing cavity receiver designs with $Q_s = 8$ kW and $C_{feed} = 18.1$ g/min	299
7.10	Performance of the optimal small-scale absorbing cavity receiver configuration at 8 kW and 1 MW	302
D.1	Results for Design 1 (2 <sup>13-8</sup> ): reflective cavity	361
D.2	Results for Design 2 (2 <sup>6-2</sup> ): reflective cavity	363
D.3	Results for Design 3 $(2^{8-4})$ : reflective cavity with 6-7 kW solar power	364
D.4	Results for Design 3 $(2^{8-4})$ : reflective cavity with 7-8 kW solar power	365
D.5	Results for Design 4 (2 <sup>4-1</sup> ): reflective cavity	366
D.6	Results for Design 5 (face-centered central composite): reflective cavity	367
D.7	Results for Design 1 (2 <sup>13-8</sup> ): absorbing cavity	369
D.8	Results for Design 2 (2 <sup>6-2</sup> ): absorbing cavity	370
D.9	Results for Design 3 (face-centered central composite): absorbing cavity	371
E.1	Base parameters for calculation of thermocouple temperature	

xiii

# LIST OF FIGURES

# Figure

Schematic diagram of existing reflective cavity receiver	5
Metal oxide water-splitting cycle	8
System boundaries for the overall conversion of heat to work via a metal oxide water splitting cycle	32
Schematic boundaries of the solar reaction process	34
Coefficient in equation 2.4 as a function of conversion for (a) ZnO reduction (equation 2.5), (b) NiFe <sub>2</sub> O <sub>4</sub> reduction (equation 2.6), (c) carbon gasification (equation 2.7), (d) water thermolysis (equation 2.8)	37
Equilibrium composition with $p = 1$ bar for (a) ZnO and (b) NiFe <sub>2</sub> O <sub>4</sub> with 5 mol Ar per mol solid reactant, (c) C + H <sub>2</sub> O and (d) H <sub>2</sub> O	38
$\eta_{abs}$ (solid lines) and $\eta_t$ (dashed lines) for (a) ZnO reduction, (b) NiFe <sub>2</sub> O <sub>4</sub> reduction and (c) carbon gasification	39
Receiver efficiency $\eta_{abs}$ (solid lines) and system efficiency (dashed lines)	40
Global coordinate system for the Monte Carlo model	47
Flow diagram for a Monte Carlo model describing solar radiation entering through the receiver window	48
Receiver configuration with dimensions in cm	48
Window and cooling plate geometry	48
Incident, reflected, and refracted ray directions	58
Receiver configurations with dimensions in cm for (a) one centered tube and (b) five staggered tubes	77
Profiles of normalized collimated solar energy flux incident on the single tube surface for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (15 x 15)$ reflective cavity; (c) $(N_{\theta} x N_{\phi}) = (5 x 5)$ absorbing cavity; (d) $(N_{\theta} x N_{\phi}) = (15 x 15)$ absorbing cavity	83
	Schematic diagram of existing reflective cavity receiver

4.3	Profiles of normalized collimated solar energy flux incident on the cavity wall surface for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) =$ $(15 x 15)$ reflective cavity; (c) $(N_{\theta} x N_{\phi}) = (5 x 5)$ absorbing cavity; (d) $(N_{\theta} x N_{\phi}) = (15 x 15)$ absorbing cavity	.85
4.4	Profiles of normalized collimated solar energy flux incident on the cavity wall for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (15 x 15)$ (15 x 15) reflective cavity	.86
4.5	Profiles of normalized collimated solar energy flux incident on the center tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ reflective cavity	.87
4.6	Profiles of normalized collimated solar energy flux incident on the front east tube wall for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (15 x 15)$ reflective cavity	.88
4.7	Profiles of normalized collimated solar energy flux incident on the back east tube wall for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (15 x 15)$ reflective cavity	.88
4.8	Profiles of normalized diffuse solar energy flux incident on the single tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ absorbing cavity	.89
4.9	Profiles of normalized diffuse solar energy flux incident on the cavity wall for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (15 x 15)$ reflective cavity; (c) $(N_{\theta} x N_{\phi}) = (5 x 5)$ absorbing cavity; (d) $(N_{\theta} x N_{\phi}) = (15 x 15)$ absorbing cavity	.90
4.10	Profiles of normalized diffuse solar energy flux incident on the center tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ absorbing cavity	.91
4.11	Profiles of normalized diffuse solar energy flux incident on the front east tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ absorbing cavity	.92
4.12	Profiles of normalized diffuse solar energy flux incident on the back east tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ absorbing cavity	.92
4.13	Profiles of normalized emitted energy flux incident on the single tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (15 x 15)$ absorbing cavity	.98

XV

4.14	Profiles of normalized emitted energy flux incident on the cavity wall for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (15 x 15)$ reflective cavity; (c) $(N_{\theta} x N_{\phi}) = (5 x 5)$ absorbing cavity; (d) $(N_{\theta} x N_{\phi}) = (15 x 15)$	00
	absorbing cavity	99
4.15	Profiles of normalized emitted energy flux incident on the center tube wall for: (a) $(N_{\theta} x N_{\phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\phi}) = (5 x 5)$ absorbing cavity	100
4.16	Profiles of normalized emitted energy flux incident on the front east tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (5 x 5)$ absorbing cavity	100
4.17	Profiles of normalized emitted energy flux incident on the back east tube wall for: (a) $(N_{\theta} x N_{\Phi}) = (5 x 5)$ reflective cavity; (b) $(N_{\theta} x N_{\Phi}) = (5 x 5)$ absorbing cavity	101
4.18	Profiles of the normalized solar energy flux incident on the (a) center tube, (b) front tube, (c) back tube from 3D MC and FV models	103
5.1	Solar flux (kW/m <sup>2</sup> ) at the window surface with an attenuator opening of (a) 100%, (b) 50%, (c) 25%	116
5.2	Coordinate system for description of ray directions at the aperture	117
5.3	Angles describing ray directions for energy incident on the entire window surface with an attenuator opening of (a) 100%, (b) 50%, (c) 25%	118
5.4	Angles describing ray direction for solar energy incident on the window between: (a) -2.86 cm $< x < -0.95$ cm, (b) 0.95 cm $< x < 2.86$ cm, (c) -0.95 cm $< x < 0.95$ cm.	119
5.5	Solar energy flux absorbed by the tubes in a horizontal plane aligned with the aperture centroid	123
5.6	Solar energy flux incident on the cavity wall in a horizontal plane aligned with the aperture centroid	123
5.7	Normalized solar energy flux absorbed by the center tube as a function of vertical position and attenuator opening	124
5.8	Solar energy flux absorbed after reflection	125
5.9	Specification of incident, reflected, and transmitted directions for semi-transparent boundaries	129

xvi

5.10	Spectral directional reflectivity of (a) aluminum and (b) quartz	134
5.11	Spectral absorption and scattering efficiency for 42 nm acetylene black particles	136
5.12	Spectral scattering phase function for 42 nm acetylene black particles	136
5.13	Spectrally averaged absorption and scattering efficiency as a function of radiation temperature	137
5.14	Spectral absorption coefficient and transmissivity for the quartz window	138
5.15	Spectrally averaged quartz transmissivity and absorption coefficient	139
5.16	Equilibrium compositions for an initially equimolar carbon/steam mixture at atmospheric pressure	147
5.17	Steam gasification reaction rate predicted by a full Langmuir-Hinshelwood kinetic expression and a simplified first order model	148
5.18	Profiles of (a) temperature (K) and (b) vertical velocity (m/s) in vertical and horizontal receiver cross-sections	162
5.19	Temperature profiles around the tube circumference at a vertical position aligned with the aperture centroid	163
5.20	Radial profiles within the center tube of (a) velocity in the vertical (y) dimension and (b) fluid temperature	164
5.21	Center tube wall and centerline fluid temperatures predicted with and without absorption of radiative energy	165
5.22	Mass fraction of C, CO and CO <sub>2</sub> in a vertical slice of the center tube	166
5.23	Radial profiles of carbon mass fraction in the center tube	167
5.24	Cumulative residence time distribution for the center tube	168
5.25	Carbon conversion and centerline fluid temperature within the center tube as a function of vertical position	169
5.26	Center tube temperature profiles obtained via a three-dimensional CFD model and a simplified plug flow solution	180
5.27	Comparison of CO mole fraction predicted with either water gas shift reaction kinetic rates or equilibrium assumption	181

xvii

5.28	Experimentally measured and theoretically predicted solar power at the secondary concentrator exit	189
5.29	Specification of solar energy inputs and losses	190
5.30	Experimentally measured temperature profiles for SiC tubes compared with the theoretical model for (a) center tube and (b) center and outer tubes	194
5.31	Experimentally measured temperature profiles for front east, front west, back east, and back west SiC tubes	196
5.32	Experimentally measured temperature profiles for Inconel tubes compared with the theoretical model for (a) center tube and (b) center and outer tubes	197
5.33	Experimentally measured temperature profiles for front east, front west, back east, and back west Inconel tubes	198
5.34	Experimental measurement and theoretical predictions of carbon conversion to CO and $CO_2$ in the center tube	200
6.1	Overview of parameters describing tube positions (method A)	223
6.2	Specification of parameters describing tube positions (method A)	224
6.3	Additional factor $\theta_c$ for tube positions specified by method B	225
6.4	Effect of $N_{max}$ on receiver efficiency from Design 1	232
6.5	Receiver efficiency from Design 1 as a function of (a) $\eta_1$ and (b) $\eta_2$	233
6.2	Receiver efficiency from Design 1 as a function of cavity wall solar absorption efficiency	234
6.3	Receiver efficiency from Design 1 as a function of average plug flow residence time	235
6.4	Receiver efficiency from Design 1 as a function of (a) average and (b) maximum carbon conversion	235
6.5	Relationship between efficiency from Design 1 and the fraction of energy lost by (a) emission and (b) conduction along tube length	236
6.10	Receiver efficiency from Design 2 as a function of tube number	239

xviii

6.11	Relationship between efficiency from Design 2 and (a) tube radius or (b) total absorber area per unit length	241
6.12	Receiver configurations corresponding to designs in Table 6.7	242
6.13	Energy flux absorbed by the center tube in a horizontal plane aligned with the aperture centroid for the configurations in Figure 6.12	243
6.14	Center tube fluid temperature in the horizontal plane aligned with the aperture centroid for the configurations in Figure 6.12	244
6.15	Receiver efficiency from Design 2 as a function of (a) $\eta_1$ and (b) $\eta_2$	245
6.16	Receiver efficiency from Design 2 as a function of average reaction conversion	246
6.17	Relationship between efficiency from Design 3 and the fraction of energy lost by (a) emission and (b) conduction along tube length	251
6.18	Solar energy incident on the cavity wall with $r_{cav} = 9.14$ cm in the absence of absorber tubes	252
6.19	Solar energy incident on the cavity wall in a horizontal plane aligned with the aperture centroid for $r_{cav} = 9.14$ cm, 7.9 cm, and 6.6 cm in the absence of absorber tubes	254
6.20	Contour plots for CCD response surface for (a) solar-to-chemical efficiency and (b) maximum absorbed solar flux $(kW/m^2)$	257
6.21	(a) Profiles of temperature (K), (b) profiles of vertical velocity (m/s) in vertical and horizontal receiver slices, and (c) profiles of center tube carbon mass fraction for the optimal reflective cavity design	259
6.22	Profiles of (a) absorbed solar flux and (b) temperature around the center tube circumference as a function of vertical position	261
6.23	Center tube front and back temperature as a function of dimensionless vertical position for 7.5 kW and 1 MW	264
7.1	Profiles of temperature (K) for both (a) absorbing cavity and (b) reflective cavity and profiles of center tube carbon mass fraction for (c) absorbing cavity and (d) reflective cavity	277
7.2	Profiles of temperature around the center tube circumference for absorbing and reflective cavity configurations	278

xix

7.3	Receiver efficiency from Design 1 as a function of (a) $\eta_1$ and (b) $\eta_2$	284
7.4	Receiver efficiency from Design 1 as a function of cavity wall solar absorption efficiency.	285
7.5	Receiver efficiency from Design 1 as a function of (a) average and (b) maximum carbon conversion	286
7.6	Receiver efficiency from Design 1 as a function of emission losses by (a) net cavity wall absorption and (b) transmission	286
7.7	Relationship between efficiency from Design 2 and (a) outer tube radius or (b) total absorber area per unit length	290
7.8	Receiver efficiency from Design 2 as a function of (a) $\eta_1$ and (b) $\eta_2$	291
7.9	Receiver efficiency from Design 2 as a function of cavity wall solar absorption efficiency.	292
7.10	Receiver efficiency from Design 2 as a function of nominal plug flow residence time at standard conditions	292
7.11	Contour plots from the CCD response surface for (a) solar-to-chemical efficiency and (b) maximum temperature (K)	297
7.12	(a) Profiles of temperature (K), (b) profiles of vertical velocity (m/s) in vertical and horizontal receiver slices, and (c) profiles of center tube carbon mass fraction for the optimal absorbing cavity design	299
7.13	Profiles of (a) absorbed solar flux and (b) temperature around the center tube circumference as a function of vertical position	300
7.14	Center tube front and back external surface temperature as a function of dimensionless vertical position for 8 kW and 1 MW	303
A.1	Ratios of characteristic times for $d_p < 100$ nm	340
A.2	Ratios of characteristic times for $d_p < 50 \ \mu m$	340
A.3	Momentum Stokes number for $d_p < 40 \ \mu m$	341
A.4	Thermal Stokes number for $d_p < 40 \ \mu m$	341
A.5	Biot number for $d_p < 30 \ \mu m$	343
A.6	Effectiveness factor for $d_p < 30 \ \mu m$	343

XX

A.7	Particle diffusivity and Schmidt number for $d_p < 100 \text{ nm}$	344
A.8	Richardson number in flow tubes	345
A.9	Reynolds number in flow tubes	346
A.10	Grashof number in cavity fluid	347
B.1	Carbon monoxide and hydrogen viscosity	349
B.2	Carbon dioxide and argon viscosity	350
B.3	Binary diffusivity of dilute carbon monoxide or hydrogen in argon	350
B.4	Carbon monoxide thermal conductivity	351
B.5	Hydrogen thermal conductivity	352
B.6	Carbon dioxide thermal conductivity	352
B.7	Argon thermal conductivity	352
D.1	Tube configurations for Design 1 $(2^{13-8})$ : reflective or absorbing cavity	362
D.2	Tube configurations for Design 2 (2 <sup>6-2</sup> ): reflective cavity	363
D.3	Tube configurations for Design 3 $(2^{8-4})$ : reflective cavity	365
D.4	Tube configurations for Design 4 $(2^{4-1})$ : reflective cavity	366
D.5	Tube configurations for Design 5 (face-centered central composite): reflective cavity	368
D.6	Tube configurations for Design 2 $(2^{6-2})$ : absorbing cavity	370
D.7	Tube configurations for Design 3 (face-centered central composite): absorbing cavity	372
E.1	Calculated difference between wall and thermocouple temperatures as a function of wall temperature, thermocouple emissivity and fluid velocity	376
E.2	Calculated difference between wall and thermocouple temperatures as a function of wall temperature, fluid velocity, and fluid temperature	376

E.3	Calculated difference between wall and thermocouple temperatures as a function of wall temperature and thermal conductivity of the thermocouple probe	.377
E.4	Theoretically predicted temperature profiles for SiC tubes compared with experimentally measured values for the center and outer tubes with errors modified to account for separation between the thermocouple junction and the tube wall.	.378
E.5	Theoretically predicted temperature profiles for Inconel tubes compared with experimentally measured values for the center and outer tubes with errors modified to account for separation between the thermocouple junction and the tube wall	.378

xxii

# **Chapter I**

# Motivation, Background, and Scope

### 1.1 Motivation and Scope

### 1.1.1 Motivation

Energy consumption in the United States alone was 98 quadrillion BTU in 2010, a value which represents a more than three-fold increase in demand from 1950 and accounts for approximately 20% of world energy consumption [1]. More than 83% of this energy was derived from non-sustainable carbonaceous fuels including petroleum, coal and natural gas, while only 8% was derived from renewable sources [1]. Despite mounting demand, utilization of renewable sources has only increased by 5 quadrillion BTU in the last 60 years with the majority of growth due to wind energy and biofuels including biodiesel and corn-derived ethanol [1]. Nearly 80% of renewable sources are derived from biofuels, wood and hydroelectric, whereas solar energy accounts for only 1% of total renewable energy consumption or 0.08% of total U.S. energy consumption [1].

While consumption of an indisputably finite energy supply appropriately generates unease regarding potential inability to meet coming demand, the current and projected future environmental impacts of unsustainable consumption habits are perhaps even more concerning. Antarctic ice cores indicate that atmospheric carbon dioxide concentration varied between 180 ppm and 300 ppm over the past 650,000 years, yet carbon dioxide concentration has increased rapidly over the past century rising to 379 ppm [2]. Likewise, global average surface temperature has risen by 0.6-1°C since 1860, even after accounting for the urban heat-island effect [3], with more than half of this increase taking place in the past 30 years and eleven of the twelve warmest years on record occurring in the past twelve years [3]. Among climate scientists this rise is almost unequivocally attributed to anthropogenic activities as similar historical increases in atmospheric carbon dioxide concentration or global mean surface temperature accompanying the end of past ices ages required 5,000 years to occur [2]. Atmospheric carbon dioxide content and surface warming have contributed to noted increases in ocean acidity, modifications in atmospheric circulation and precipitation patterns, and melting of polar ice caps along with the associated rise in sea level [4].

Clearly current fossil fuel consumption practices are not only unsustainable, but produce tremendously damaging environmental and geopolitical consequences. With rapidly escalating world energy demands originating from developing countries it is perhaps unrealistic to rely purely on conservation and hope for dwindling consumption to resolve this predicament. Strategies combining conservation, improvements in energy efficiency, application of new technologies to traditional energy sources, and utilization of renewable sources must be sought. Exploitation of renewable resources, currently representing only 8% of total U.S. consumption and 6% of total world consumption [5], will be crucial. Solar energy in particular appears to possess largely untapped potential to transform the current energy landscape. Discounting that reflected or absorbed by clouds and the atmosphere, an average of 86,000 TW of solar energy arrives at the earth's surface [6]. Thus the quantity of energy reaching the earth's surface in a mere two hours of time exceeds global yearly consumption of 496 quadrillion BTU [5]. Harnessing just 0.01% of the solar energy reaching the earth's surface in a given year would address more than half of global energy demand. Yet capturing this energy and converting it to a useful form proves difficult as it reaches the earth's surface with flux densities of, at best, on the

order of 1 kW/m<sup>2</sup> and is characterized by an inherently diffuse and intermittent nature even during daylight hours. Furthermore, and not coincidentally, locations possessing ideal solar resources frequently do not overlap geographically with population centers. Thus solar energy must ideally be captured and stored in a transportable form.

One of many suggested solutions is the utilization of concentrated solar energy to drive highly endothermic chemical reactions. Both hydrogen producing thermochemical cycles and solar gasification of carbonaceous fuels, among other processes, allow for storage of solar energy in the bonds of chemical reaction products, thereby circumventing challenges associated with the diffuse and transient nature of solar power. Ideal locations for concentrating solar, characterized by high incidence of direct normal radiation, are distributed globally and can be found in various regions across Africa, Asia, the Middle East, Australia, and South America as well as in the southwest United States [1, 7]. A 24-35% solar to hydrogen efficiency based on the higher heating value (HHV) of reaction products has been estimated for various metal oxide thermochemical cycles assuming negligible optical losses related to the solar concentrating system [8-11]. This translates into roughly 19-29% efficiency for converting solar heat to usable work in an ideal fuel cell [8, 10, 11]. Including a 60% optical efficiency for the solar collection system, the solar to hydrogen HHV efficiency is reduced to 15-25% [9, 11-13]. Conventional low temperature electrolysis with electricity produced using concentrated solar energy typically results in at best 14-19% solar to hydrogen HHV efficiency [12, 13] and thus hydrogen production via thermochemical cycles appears to offer a theoretical advantage over more traditional technologies.

Introduction of a solar energy source to conventional steam gasification processes for carbonaceous materials upgrades the calorific value of the feedstock by 30-45% [14]. Solar

gasification of coal, including downstream water-gas shift and CO<sub>2</sub>/H<sub>2</sub> separation, yields approximately 70% conversion of solar energy and original fuel HHV to usable work in an ideal fuel cell [10, 15] neglecting optical losses from the concentration system. If the syngas product is used to generate electricity through conventional means such as a gas turbine or combined cycle, the solar coal gasification process results in a 30-50% reduction in CO<sub>2</sub> emissions compared to conventional coal-fueled Rankine cycles [10, 14]. Though these studies have been carried out for non-sustainable carbonaceous feedstocks, substitution of cellulosic biomass for coal renders the gasification process both carbon-neutral and renewable. Economical assessments indicate that solar thermochemical hydrogen production can be competitive with water electrolysis [10].

Yet the above assessments are wholly contingent on the existence of a solar receiver which can effectively capture the supplied solar energy in the chemical products. It is estimated that optical components of the solar concentration system for a full-scale plant can account for as much as 50-80% of initial capital costs [16], thus the possibility of any solar-thermal process generating an economically feasible alternative to fossil fuels hinges on the effectiveness of the receiver. Receiver design has typically been carried out on a principally empirical basis leading to systems detailed in the literature which rarely exceed a solar-to-chemical efficiency of 10% on a 10 kW laboratory scale. Understanding the behavior of these solar receiver / chemical reactor systems on the basis of fundamental transport phenomena driving the process is essential to improving both receiver design and performance.

#### 1.1.2 Scope

The primary objectives of this work were to develop a fundamental understanding of heat and radiation transport processes occurring within a type of closed cavity solar aerosol flow reactor, and to apply this understanding to ascertain efficiency limitations and factors driving efficiency, with the aim of moving from a largely empirical to a more fundamental theoretical approach for solar receiver design. The first step in achieving these goals was to develop an accurate model of all applicable heat, mass, momentum and radiation transport processes occurring in an existing prototype indirectly-irradiated reflective cavity receiver depicted in Figure 1.1. The existing receiver consists of a cylindrical, reflective polished aluminum cavity with a windowed or windowless aperture enclosing an array of five tubes. In the current study it was operated in an aerosol flow configuration with a fluid/particle mixture flowing through each tube.



Figure 1.1: Schematic diagram of existing reflective cavity receiver

Computational fluid dynamics techniques were used to solve fundamental heat, mass, and momentum transport equations in a three-dimensional steady state model of the existing receiver. The inherent complexity of the integro-differential equations governing radiative heat transfer restricts analytical solutions to only the simplest of scenarios. A number of approximate methods including surface exchange or radiosity, finite volume or discrete ordinates, and statistical Monte Carlo methods have been developed, each with drawbacks related to solution accuracy, computational requirements, and ability to couple with detailed convective and conductive heat transfer models. Use of the finite volume method to solve the radiative transfer equation was appealing because of its compatibility with detailed control-volume based computational fluid dynamics techniques. However, in light of previous studies, accuracy of the finite volume method was at best questionable for the receiver geometry of interest and was evaluated in comparison to Monte Carlo solutions with the goal of proposing a modeling strategy for transport of radiative energy that was both sufficiently accurate and computationally efficient.

Accurate depiction of receiver performance required treatment of both physical phenomena and chemical reaction phenomena occurring within the tubes. The focus of the current work was on the performance of the receiver and, as such, the chemical process may be any of a variety of highly endothermic reactions including thermal reduction of a number of metal oxide species, or gasification of carbonaceous materials including biomass or biomass char. However, detailed knowledge of the kinetic mechanism and intrinsic surface reaction rate at elevated temperatures was critical to accurate prediction of receiver performance. Biomass pyrolysis and gasification reaction schemes and kinetic parameters at high temperatures are extremely complex and poorly understood and thus, for the purposes of this study, it was advantageous to employ gasification of pure carbon as a simplified test reaction thereby taking advantage of the large body of literature discussing gasification of low-ash coal char and petcoke.

Validation was accomplished through comparison of computational model results with experimental data collected on-sun using the existing receiver. Receiver models were experimentally validated under both inert and reactive conditions with tubes constructed from either high temperature metal alloys or ceramic materials. This model was then utilized to characterize the performance of the current receiver under a variety of conditions and to investigate the impacts of various parameters describing receiver configuration and operating conditions. Information gained through these computational studies suggested strategies for improving both design and performance on the basis of the fundamental transport phenomena occurring in the closed-cavity receiver. These studies were carried out for both a reflective cavity configuration and an industrially-relevant absorbing cavity configuration with optimal designs identified on the basis of maximal solar-to-chemical receiver efficiency. Various studies suggest that process economics are governed predominantly by the optical components comprising the concentrating system, and thus receiver optimization on the basis of solar energy utilization mirrors economic optimization. It is expected that optimal receiver designs for carbon and biomass gasification will possess similar features given the analogous temperature range under which the reactions proceed. A similar procedure could be followed for additional chemical processes by inserting a modified reaction or fluid/particle flow model into the framework of the heat, mass, momentum and radiation models developed for the carbon gasification reaction. Thus while this study carried out calculations identifying optimal designs specifically for the carbon gasification reaction, the procedure provides the framework through which receiver design may be optimized for any chemistry on the basis of the fundamental transport phenomena occurring within the receiver.

### **1.2 Background and Literature Review**

#### 1.2.1 Solar-thermal processes

Concentrated solar energy can be used to provide the heat necessary to drive various highly endothermic chemical reactions for renewable fuel production including direct thermolysis of water, thermal reduction of metal oxides for production of hydrogen from water splitting cycles, carbothermal reduction of metal oxides, thermal decarbonization or cracking of methane, and gasification of cellulosic biomass, coal or other carbonaceous materials to produce synthesis gas [8, 10, 14, 17]. Direct thermolysis of water is typically infeasible as temperatures exceeding 2500 K are required, necessitating high concentration ratios, exotic materials for receiver construction, and effective high temperature gas separation techniques for hydrogen and oxygen produced in a single reaction step [14, 18-20]. Multi-step reaction sequences have been proposed as an alternative to direct thermolysis in order to reduce the requisite temperature and eliminate the need for high temperature gas separations [8, 10, 14, 21, 22]. Metal oxide cycles involve thermal reduction of a metal oxide and utilize concentrated solar energy or, in limited cases, nuclear waste heat to provide the energy necessary to carry out the highly endothermic chemical reaction. The reduced metal or metal oxide is then reacted with steam to produce hydrogen and regenerate the original starting material, and the net effect is the production of hydrogen and oxygen from water in discrete steps. A simplified schematic of this process is illustrated in Figure 1.2.



Figure 1.2: Metal oxide water-splitting cycle

Candidate metal oxides have a reduction temperature substantially below that required for the direct thermolysis of water and materials including ZnO [11, 23-25],  $Mn_2O_3$  [26-28],  $SnO_2$  [29, 30], CeO<sub>2</sub> [31-33], and mixed iron oxides of the form  $M_xFe_{3-x}O_4$  where M typically represents Co, Ni, Mn, Zn or Fe [34-40] have been investigated extensively in the literature with reduction temperatures typically ranging between 1700-2200 K. Ongoing work seeks to address challenges related to an excessively high reduction temperature, the necessity of rapidly quenching volatile reaction products to prevent recombination, sintering and loss of active surface area during high temperature cycling, kinetic or thermodynamic limitations on the oxidation step, and identification of receiver materials not only tolerant of a high-temperature oxidizing environment, but also sufficiently resistant to the thermal stresses imposed by the inherently transient nature of the concentrated solar input [10, 14, 24].

Gasification of cellulosic biomass, coal, or other carbonaceous materials with steam or  $CO_2$  is represented in generic form in equation 1.1 and typically carried out at a comparatively lower temperature than the metal oxide cycles described above.

$$C_{x}H_{y}O_{z} + (x-z)H_{2}O \rightarrow \left(\frac{y}{2} + x - z\right)H_{2} + xCO \qquad (1.1)$$

The mixture of CO and  $H_2$ , known as synthesis gas or "syngas", generated by the gasification reaction can be reformed into various liquid fuels, ammonia, hydrogen, or a number of commodity chemicals by Fischer-Tropsch type processes. Traditional autothermal gasification processes proceed with partial combustion of the feedstock supplying the necessary heat for the endothermic gasification reaction, resulting in both CO<sub>2</sub> emissions and practical limitations on the operating temperature as combustion of up to 30% of the biomass feedstock may be required to sustain an elevated temperature [41]. Gasification processes at comparatively lower temperature result in formation of volatile condensable hydrocarbons and aromatics commonly referred to as tar [42-45] leading to fouling of downstream catalytic surfaces. Solar energy has been proposed as an alternative means of providing the process heat [41, 46-48]. Introduction of solar energy to the gasification process eliminates the necessity of feedstock combustion and upgrades the calorific value of the feedstock by storing solar energy in chemical bonds of the reaction products. Comparatively higher temperatures are achievable resulting in reduction or elimination of tar production [42, 43]. Yu et al. [49] reported a 40% decrease in tar formation at 900°C compared to 700°C, whereas Lichty et al. noted clearly diminished tar production at 1200°C compared to 1000°C [50].

#### 1.2.2 Design and efficiency of current receivers

Metal oxide cycles and biomass gasification, when powered by the clean energy of the sun, are theoretically entirely renewable and carbon neutral. Yet the inherent advantages of these processes cannot be exploited on a large scale without detailed knowledge and fundamental understanding of the solar receiver. Numerous solar reactor concepts have been proposed in the literature [50-63] with most consisting of cavity-receiver type designs in which concentrated solar radiation enters into a closed cavity through a small aperture or window. Receiver cavities are typically constructed from strongly absorbing materials and insulated heavily so as to minimize radiative absorption and conduction losses. High temperature oxidizing environments commonly require the use ceramic materials which are poorly resistant to thermal shock and often result in cracking of receiver walls or insulating materials during on-sun operation [52, 64]. Reflective cavity receivers are subject to increased conduction losses as walls must remain sufficiently cool to maintain the quality of the reflective surface, and are only feasible in indirectly-irradiated designs without the possibility of particle contact. Nevertheless, the small

thermal mass of reflective cavity receivers makes them amenable to laboratory scale experimental operation.

Many receiver concepts are directly irradiated designs in which reactants are exposed directly to concentrated solar radiation [51, 54, 55, 58, 60-63]. Rapid and efficient heating is possible owing to direct absorption of solar energy by reactant particles, and these designs have the potential to minimize solar load on the receiver walls [14]. However, these designs tend to exhibit considerable heat losses by particle emission and necessitate the presence of a transparent quartz window presenting complications related to particle fouling, severe gas environments, and potential for large-scale designs. Vortex flow patterns, an inert sweep gas, or a rotating cavity are typically employed to prevent particle contact with and deposition on the transparent window surface. Not only do these methods enhance convective heat losses and increase the mechanical complexity of the design, but despite these efforts, particle deposition on the window surface often remains a problem during experimental testing [65, 66].

Indirectly irradiated designs can eliminate the need for a transparent window by enclosing reactants in either opaque absorbing tubes or a separate cavity [50, 52, 53, 56, 57, 59]. Absorption by the tube or cavity material and subsequent emission is required to heat the reactant species, providing an additional mechanism for heat loss as tube or cavity materials must possess a high enough thermal conductivity to withstand thermal shock. Dual-cavity designs consist of an upper and lower cavity, with the upper cavity devoid of reactant particles and constructed of a highly absorbing material possessing desirable thermal shock properties such as graphite or silicon carbide [57, 67, 68]. Solar energy is absorbed by the walls of the upper cavity and re-emitted to a lower cavity containing reactant particles. Compared to these dual-cavity receivers, designs with aerosol flow tubes offer the advantage of improved heat and

mass transfer rates due to high surface area to volume ratios characterizing small particles entrained in a transport gas [25, 59, 69]. As a result rapid heating rates and kinetically controlled reactions are achievable [59, 70], allowing for short residence times and high throughput of reactants. Furthermore, indirectly irradiated configurations with aerosol flow tubes tend to have mechanically simplistic and stationary designs, a considerable benefit in view of the elevated operating temperatures and inherently transient nature of the solar power source.

Receivers detailed in the literature are generally designed initially with little fundamental basis leading to inadequacies including low efficiency and highly non-uniform heating. Receiver solar-to-chemical efficiency is calculated from equation 1.2 where the numerator represents the enthalpy change for the process converting the reactants at the inlet temperature to the products at the temperature attained in the receiver.

$$\eta = \frac{\Delta H|_{\text{reactants}(T_{inlet}) \to \text{products}(T)}}{Q_{solar}}$$
(1.2)

Predicted efficiencies for designs accepting under 10 kW solar power are typically in the range of 1-10% with heat losses primarily due to emission out of the transparent window (30-55% of  $Q_{solar}$ ) and conduction (30-65% of  $Q_{solar}$ ) [53, 58-60, 64, 67, 69, 71]. Receiver cavities are either constructed out of a high temperature refractory material and insulated [51-53, 57, 58, 60, 62, 67, 72] or constructed from a metallic material and actively cooled or shielded from solar energy by reactant particles [50, 55, 63, 73]. Conduction losses at the cooled quartz window can be substantial even when the cavity walls are heavily insulated [51, 71, 74]. Radiation losses remain relatively unaffected by the size scale of the receiver; however, simplified computational models of existing insulated cavity receivers predict that conduction losses may decrease to under 10% of the solar input when the design is scaled to accept a solar input of 1 MW [69, 71]. Efficiency for these large-scale designs has been approximated from simplified heat transfer models and predictions range from 5-50% for solar power inputs on the order of 1-10 MW [58, 69, 71, 72], though the simplified models used to generate these estimates have not been validated at this scale.

#### 1.2.3 Transport and radiation modeling

Designing an effective receiver entails optimizing heat input to the reactants and matching the kinetic rate and energy requirements for the chemical reaction to the solar input, while minimizing both conductive and radiative losses. Computational models are commonly used to predict tube or cavity temperatures along with corresponding reactant conversions or receiver efficiency, and accurate models can be used to facilitate the design of highly effective receivers. Comprehensive treatment of receiver transport phenomena involves coupling typical momentum, continuity, and energy equations with reaction kinetics and the integro-differential The inherent complexity of the equations governing equations describing radiative transfer. radiative heat transfer restricts analytical solutions to the simplest scenarios often involving graydiffuse surfaces and either non-attenuating or isotropically scattering media with negligible spectral and directional dependence of all optical properties. Finite volume or discrete ordinates, [51, 74-78], radiosity, [55, 57, 79, 80] and Monte Carlo [56, 58, 60, 69, 81-84] methods or related combinations [71, 72, 85] are commonly employed to solve the radiative transfer Radiosity methods are restricted to problems with non-participating media [86] problem. whereas Monte Carlo, finite volume and discrete ordinates methods are fully capable of treating absorbing, emitting, anisotropically scattering non-gray media in complex geometries [86-91].

Monte Carlo (MC) methods apply probabilistic models for radiative phenomena [86, 87] and allow for straightforward incorporation of both spectral and directional optical properties.

The energy leaving a surface is described by a stochastic number of bundles of energy or rays with direction and wavelength corresponding to the physical laws governing radiation exchange. The subsequent sequence of absorption, reflection, or emission events at boundary walls and within the participating media follows the principles governing Markov chains with each event occurring entirely independently of previous events. Solutions obtained via MC methods are not subject to discretization errors and are frequently used to obtain benchmark calculations [86, 87] though such calculations may be computationally intensive, particularly for systems with strongly participating media. While these solutions are highly accurate within a statistical limit, they are not directly compatible with control-volume based computational fluid dynamics (CFD) approaches. In solar receiver modeling studies, use of the MC technique typically comes at the expense of complexity in the treatment of fluid flow and heat transfer equations, which are commonly simplified to one-dimensional or global/macroscopic models with constant properties [58, 60, 69, 72, 81, 83, 84, 92].

The finite volume (FV) [88, 89] and discrete ordinates (DO) [90, 91] methods for radiative heat transfer are appealing as they are capable of treating non-isothermal, absorbing, emitting, anisotropically scattering, non-gray media in complex geometries while retaining compatibility with a control volume based computational fluid dynamics modeling approach [88]. The finite volume method integrates the radiative transfer equation (equation 1.3) [86] over both control volumes and finite solid angles  $\omega^l$  to yield a set of discretized transport equations for the radiative intensity within each finite solid angle [88, 89].

$$\frac{dI(r,s)}{ds} = -(a+\sigma_s)I(r,s) + aI_b(r) + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r,s')\Phi(s,s')d\omega'$$
(1.3)

Using this method the radiative transfer equation can be solved simultaneously and, in principal, on the same spatial mesh as fundamental heat, mass and momentum transport equations leading
to close coupling between solutions for radiative energy and surface temperatures. Thus FV or DO radiation models are commonly implemented in receiver modeling studies in conjunction with highly complex three-dimensional fluid flow and heat transfer models including, for instance, discrete particle models, turbulence, and the effects of buoyancy [51, 74-78, 85]. However, previous studies have detailed various maladies, namely ray effects and false scattering errors, that afflict the solutions of finite volume based methods and whose effects can be both problematic and difficult to eliminate [93, 94]. These errors are particularly pronounced for cases with weakly participating or non-participating media, isolated heat sources, specularly reflective enclosure surfaces, and collimated radiation [93, 95-98] calling into question the applicability of FV or DO methods for solar receivers which commonly involve an isolated, strongly directionally dependent energy source with non-participating cavity media in indirectlyirradiated designs. Ray effects originate from the approximation of a continuum angular distribution with a finite set of directions and can never be completely eliminated from finite volume solutions. False scattering, on the other hand, draws analogies with false diffusion in the CFD community and results from spatial discretization techniques. Ray effects, or ray concentration errors, were originally identified in discrete ordinates equations [99] and were later found to be present in finite volume solutions as well [94]. While many past studies quantifying errors in FV and DO solutions have been carried out for grey enclosures with absorbing/emitting/scattering media and diffusely emitted radiation, relatively few have been performed for highly specularly reflective enclosures with the collimated or strongly directionally-dependent intensity distributions that typically result from solar concentrating systems.

16

A number of studies have investigated the accuracy of variations of the DO and FV methods in enclosures with partially heated surfaces [93-98, 100-102]. Enclosure walls are typically black or gray and diffuse, while emitted or incident radiation is either diffuse or collimated. Ray effects commonly produce oscillations in heat flux solutions and, while never completely eliminated, can be alleviated by increasing the number of ordinate directions (DO) or minimizing solid angle extents (FV). However, ray effect errors are not always evidenced by oscillatory solutions and may also be present in smooth profiles. In enclosures with partially heated walls, ray effects are most pronounced for a localized or isolated heat source and worsen as either the heated length [95-97, 100] or the optical thickness [93, 95, 100] of the medium decreases. Koo et al. [98] found that oscillations in the solutions of DO equations may be more severe when enclosure walls are highly reflective. Various methods to minimize ray effects have been proposed, but these methods often either fail to universally eliminate errors in cases with isolated heat sources or cannot be applied to complex geometries [100]. False scattering arises from approximation of intensity values at control volume faces with the surrounding nodal values and tends to produce a general smearing of the intensity field. Errors due to false scattering can be reduced through the use of smaller control volumes and higher order spatial discretization schemes, though the use of higher order discretization schemes may, in some cases, induce oscillations independent of those originating from ray effects [93, 94, 96, 101, 102].

#### 1.2.4 Modeling gasification kinetics

The receiver model must couple heat, mass, momentum and radiation transport models with an accurate depiction of chemical reaction kinetics. Steam gasification of a biomass feedstock can be broken into separate processes of pyrolysis or devolatilization and char gasification. Pyrolysis is nearly instantaneous at high temperatures and generally considered to be heat transfer limited, particularly for rapid heating rates [41, 103-107]. Lack of separation between intrinsic kinetic rates and transport effects leads to wide variation in kinetic parameters reported in the literature [41, 44, 103, 108]. As such, a consensus on pyrolysis kinetics has not yet been reached [103, 109] and no pyrolysis models exist that are capable of satisfactorily predicting product yields over wide ranges of conditions and feedstocks [110]. Availability of pyrolysis and gasification rates at high temperature is particularly limited in the literature [44].

Gasification kinetics can be strongly dependent on pyrolysis conditions, even when pyrolysis is not directly included in the kinetic study. Along with influencing the distribution of char and tar formed in the reactor, pyrolysis conditions affect char reactivity with rapid heating rates producing a highly reactive char structure characterized by a large volume of macropores [104, 111, 112]. Biomass char tends to exhibit reactivity greater than that of typical coal chars attributable to comparatively higher porosity, larger pores, and increased inorganic material content [111]. Models for biomass char gasification exhibit substantial variability in both the description of the intrinsic surface reaction and in the complexity of associated particle properties and heat or mass transfer effects [44, 104, 106, 107, 111, 113-116]. Fundamentally realistic kinetic models of char gasification require intrinsic surface kinetics and knowledge of chemical structure, inorganic constituents, porosity, and reactive surface area; however, even models including all of these details commonly produce char reactivities varying by up to four orders of magnitude [111]. Intrinsic surface gasification rates are heavily influenced by constituent inorganic material which is believed to have a catalytic effect. Activation energies measured for coal chars with minimal inorganic material can exceed those evaluated for materials with substantial inorganic content by 100 kJ/mol [111]. Variations in porous structure

and reactive surface area are known to impact predicted kinetic parameters, but are difficult to assess and are thus commonly simplified to empirical correlations [117, 118]. Consequently, comparison of complex models with experimental data often proves challenging and most models reported in the literature are simplified global reactivity descriptions [111, 114]. Though these global models are frequently utilized in combination with heat and mass transfer models of chemical reactors [44, 115, 119], published reaction models lump intrinsic chemical phenomena with physical processes [114] thereby producing apparent parameters with at best limited applicability to disparate materials and conditions. The introduction of a radiative energy source presents additional challenges associated with rapidly varying optical properties as the weakly absorbing unreacted biomass is transformed into strongly absorbing char particles [41].

Gasification kinetics for pure carbon, low-ash coal chars and petcoke are comparatively simpler. The carbon-steam surface reaction is typically presumed to follow either an oxygen-exchange or hydrogen-inhibition mechanism. The oxygen-exchange mechanism consists of dissociative reversible adsorption of steam on the carbon surface followed by irreversible combination of adsorbed oxygen atoms with surface carbon [111, 116, 120-124]. The hydrogen-inhibition mechanism is based on irreversible dissociative steam adsorption, reversible hydrogen adsorption, and irreversible combination of adsorbed oxygen inhibition differs in each mechanism, both lead to an identical Langmuir-Hinshelwood type rate expression. Many other mechanisms have been suggested [121, 125] including those applicable for combined CO<sub>2</sub>/H<sub>2</sub>O gasification [122] or gasification at elevated pressures [126]. At low partial pressures the effect of hydrogen inhibition is commonly neglected such that the Langmuir-Hinshelwood rate expression can be condensed into a simple n<sup>th</sup> order global model [111, 121].

#### 1.2.5 Receiver optimization

Improvements in receiver efficiency produced by scaling a fixed geometry from 5-10 kW to 1-10 MW have been examined via various computational studies [58, 69, 71, 72, 127]. Yet only a limited number of studies detailed in the literature explore the impact of receiver size, tube configuration, or operating conditions on receiver efficiency at a fixed scale [75, 128-130]. These studies are based on simplified receiver models which may not accurately depict all relevant physical and chemical processes. Tescari et al. examined a receiver in which reactive material affixed around vertical cylindrical walls was heated via direct absorption of solar energy introduced at the top end of the cylinder [128, 129]. The impact of a shape factor and cylinder void fraction were investigated by means of a constructal optimization method intended to approximate the tendency of geometric variations in the realistic system based on that predicted for a substantially simplified problem. An algebraic model of receiver efficiency was developed and derived from simple macroscopic energy balances for individual reactor segments. Melchior et al. examined radiative transfer and surface temperature profiles in a perfectly insulated absorbing cavity reactor via a Monte Carlo model and macroscopic surface energy balances neglecting convective and conductive heat transfer [130]. The optimal distance between a single tube and the aperture was investigated along with tube configuration for arrays consisting of two, four, or eight tubes on the basis of maximum and average tube temperatures in the absence of chemical reaction. Haussener et al. considered a two-dimensional slice of an indirectly irradiated multiple tube receiver with absorbing cavity walls for thermal reduction of ZnO via a simplified computational fluid dynamics heat transfer model combined with a finite volume treatment of solar and emitted radiative energy [75]. Variations in solar concentration, number of tubes, tube size, ZnO feed rate, window aspect ratio and cavity size were taken into

consideration with ZnO feed rate and tube number producing the largest impact on predicted receiver efficiency.

## References

- 1. *Annual Energy Review 2010.* 2011: U.S. Energy Information Administration, Washington DC.
- Jansen, E., Overpeck, J., Briffa, K.R., Duplessy, J., Joos, F., Masson-Delmotte, V., Olago, D., Otto-Bliesner, B., Peltier, W.R., Rahmstorf, S., Ramesh, R., Raynaud, D., Rind, D., Solomina, O., Villalba, R., and Zhang, D., *Palaeoclimate*, in *Climate Change* 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, S. Soloman, D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Avery, M. Tignor, and H.L. Miller, Editors. 2007, Cambridge University Press: Cambridge.
- 3. Trenberth, K.E., Jones, P.D., Ambenje, P., Bojariu, R., Easterling, D., Klein Tank, A., Parker, D., Rahimzadeh, F., Renwick, J.A., Rusticucci, M., Soden, B., and Zhai, P., Observations: Surface and Atmospheric Climate Change, in Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, S. Soloman, D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Avery, M. Tignor, and H.L. Miller, Editors. 2007, Cambridge University Press: Cambridge.
- Bindoff, N.L., Willebrand, J., Artale, V., Cazenave, A., Gregory, J., Gulev, S., Hanawa, K., Le Quere, C., Levitus, S., Nojiri, Y., Shum, C.K., Talley, L.D., and Unnikrishnan, A., Observations: Oceanic Climate Change and Sea Level, in Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, S. Soloman, D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Avery, M. Tignor, and H.L. Miller, Editors. 2007, Cambridge University Press: Cambridge.
- 5. Marban, G. and Vales-Solis, T., Towards the hydrogen economy? *International Journal of Hydrogen Energy*, 2007. **32**(12): p. 1625-1637.
- 6. Hermann, W.A., Quantifying global exergy resources. *Energy*, 2006. **31**(12): p. 1685-1702.
- 7. Assessment of the World Bank Group / GEF Strategy for the Market Development of Concentrating Solar Thermal Power. 2006: World Bank, Washington DC.
- 8. Kodama, T. and Gokon, N., Thermochernical cycles for high-temperature solar hydrogen production. *Chemical Reviews*, 2007. **107**(10): p. 4048-4077.

- 9. Martinek, J., Channel, M., Lewandowski, A., and Weimer, A.W., Considerations for the Design of Solar-Thermal Chemical Processes. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(3).
- 10. Steinfeld, A., Solar thermochemical production of hydrogen a review. *Solar Energy*, 2005. **78**(5): p. 603-615.
- 11. Steinfeld, A., Solar hydrogen production via a two-step water-splitting thermochemical cycle based on Zn/ZnO redox reactions. *International Journal of Hydrogen Energy*, 2002. **27**(6): p. 611-619.
- 12. Pregger, T., Graf, D., Krewitt, W., Sattler, C., Roeb, M., and Moller, S., Prospects of solar thermal hydrogen production processes. *International Journal of Hydrogen Energy*, 2009. **34**(10): p. 4256-4267.
- 13. Kolb, G. and Diver, R.B., *Screening Analysis of Solar Thermochemical Hydrogen Concepts*. 2008, Sandia National Laboratories: Albuquerque, New Mexico.
- 14. Kodama, T., High-temperature solar chemistry for converting solar heat to chemical fuels. *Progress in Energy and Combustion Science*, 2003. **29**(6): p. 567-597.
- 15. Steinfeld, A. and Weimer, A.W., Thermochemical Production of Fuels with Concentrated Solar Energy. *Optics Express*, 2010. **18**(9): p. A100-A111.
- Steinfeld, A. and Spiewak, I., Economic evaluation of the solar thermal CO-production of zinc and synthesis gas. *Energy Conversion and Management*, 1998. **39**(15): p. 1513-1518.
- 17. Fletcher, E.A., Solarthermal processing: A review. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2001. **123**(2): p. 63-74.
- Kogan, A., Direct solar thermal splitting of water and on-site separation of the products -II. Experimental feasibility study. *International Journal of Hydrogen Energy*, 1998.
   23(2): p. 89-98.
- 19. Kogan, A., Direct solar thermal splitting of water and on-site separation of the products IV. Development of porous ceramic membranes for a solar thermal water-splitting reactor. *International Journal of Hydrogen Energy*, 2000. **25**(11): p. 1043-1050.
- 20. Kogan, A., Spiegler, E., and Wolfshtein, M., Direct solar thermal splitting of water and on-site separation of the products. III. Improvement of reactor efficiency by steam entrainment. *International Journal of Hydrogen Energy*, 2000. **25**(8): p. 739-745.
- 21. Abanades, S., Charvin, P., Flamant, G., and Neveu, P., Screening of water-splitting thermochemical cycles potentially attractive for hydrogen production by concentrated solar energy. *Energy*, 2006. **31**(14): p. 2805-2822.

- 22. Perkins, C. and Weimer, A.W., Likely near-term solar-thermal water splitting technologies. *International Journal of Hydrogen Energy*, 2004. **29**(15): p. 1587-1599.
- Palumbo, R., Lede, J., Boutin, O., Ricart, E.E., Steinfeld, A., Moller, S., Weidenkaff, A., Fletcher, E.A., and Bielicki, J., The production of Zn from ZnO in a high-temperature solar decomposition quench process - I. The scientific framework for the process. *Chemical Engineering Science*, 1998. 53(14): p. 2503-2517.
- 24. Keunecke, M., Meier, A., and Palumbo, R., Solar thermal decomposition of zinc oxide: an initial investigation of the recombination reaction in the temperature range 1100-1250K. *Chemical Engineering Science*, 2004. **59**(13): p. 2695-2704.
- 25. Perkins, C., Lichty, P.R., and Weimer, A.W., Thermal ZnO dissociation in a rapid aerosol reactor as part of a solar hydrogen production cycle. *International Journal of Hydrogen Energy*, 2008. **33**(2): p. 499-510.
- 26. Sturzenegger, M., Ganz, J., Nuesch, P., and Schelling, T., Solar hydrogen from a manganese oxide based thermochemical cycle. *Journal De Physique Iv*, 1999. **9**(P3): p. 331-335.
- 27. Sturzenegger, M. and Nuesch, P., Efficiency analysis for a manganese-oxide-based thermochemical cycle. *Energy*, 1999. **24**(11): p. 959-970.
- 28. Francis, T.M., Lichty, P.R., and Weimer, A.W., Manganese oxide dissociation kinetics for the Mn2O3 thermochemical water-splitting cycle. Part 1: Experimental. *Chemical Engineering Science*, 2010. **65**(12): p. 3709-3717.
- 29. Abanades, S., Charvin, P., Lemont, F., and Flamant, G., Novel two-step SnO2/Sno watersplitting cycle for solar thermochemical production of hydrogen. *International Journal of Hydrogen Energy*, 2008. **33**(21): p. 6021-6030.
- 30. Charvin, P., Abanades, S., Lemont, F., and Flamant, G., Experimental study of SnO2/SnO/Sn thermochemical systems for solar production of hydrogen. *Aiche Journal*, 2008. **54**(10): p. 2759-2767.
- 31. Abanades, S. and Flamant, G., Thermochemical hydrogen production from a two-step solar-driven water-splitting cycle based on cerium oxides. *Solar Energy*, 2006. **80**(12): p. 1611-1623.
- 32. Chueh, W.C., Falter, C., Abbott, M., Scipio, D., Furler, P., Haile, S.M., and Steinfeld, A., High-Flux Solar-Driven Thermochemical Dissociation of CO(2) and H(2)O Using Nonstoichiometric Ceria. *Science*, 2010. **330**(6012): p. 1797-1801.
- 33. Abanades, S., Legal, A., Cordier, A., Peraudeau, G., Flamant, G., and Julbe, A., Investigation of reactive cerium-based oxides for H(2) production by thermochemical two-step water-splitting. *Journal of Materials Science*, 2010. **45**(15): p. 4163-4173.

- 34. Nakamura, T., Hydrogen Production from Water Utilizing Solar Heat at High-Temperatures. *Solar Energy*, 1977. **19**(5): p. 467-475.
- 35. Kodama, T., Kondoh, Y., Yamamoto, R., Andou, H., and Satou, N., Thermochemical hydrogen production by a redox system of ZrO2-supported Co(II)-ferrite. *Solar Energy*, 2005. **78**(5): p. 623-631.
- 36. Allendorf, M.D., Diver, R.B., Siegel, N.P., and Miller, J.E., Two-Step Water Splitting Using Mixed-Metal Ferrites: Thermodynamic Analysis and Characterization of Synthesized Materials. *Energy & Fuels*, 2008. **22**(6): p. 4115-4124.
- 37. Scheffe, J.R., Li, J.H., and Weimer, A.W., A spinel ferrite/hercynite water-splitting redox cycle. *International Journal of Hydrogen Energy*, 2010. **35**(8): p. 3333-3340.
- Tamaura, Y., Steinfeld, A., Kuhn, P., and Ehrensberger, K., Production of Solar Hydrogen by a Novel, 2-Step, Water-Splitting Thermochemical Cycle. *Energy*, 1995. 20(4): p. 325-330.
- 39. Charvin, P., Abanades, S., Flamant, G., and Lemort, F., Two-step water splitting thermochemical cycle based on iron oxide redox pair for solar hydrogen production. *Energy*, 2007. **32**(7): p. 1124-1133.
- 40. Agrafiotis, C., Roeb, M., Konstandopoulos, A.G., Nalbandian, L., Zaspalis, V.T., Sattler, C., Stobbe, P., and Steele, A.M., Solar water splitting for hydrogen production with monolithic reactors. *Solar Energy*, 2005. **79**(4): p. 409-421.
- 41. Lede, J., Solar thermochemical conversion of biomass. *Solar Energy*, 1999. **65**(1): p. 3-13.
- Han, J. and Kim, H., The reduction and control technology of tar during biomass gasification/pyrolysis: An overview. *Renewable & Sustainable Energy Reviews*, 2008. 12(2): p. 397-416.
- 43. Devi, L., Ptasinski, K.J., and Janssen, F.J.J.G., A review of the primary measures for tar elimination in biomass gasification processes. *Biomass & Bioenergy*, 2003. **24**(2): p. 125-140.
- 44. Brown, A.L., Dayton, D.C., Nimlos, M.R., and Daily, J.W., Design and characterization of an entrained flow reactor for the study of biomass pyrolysis chemistry at high heating rates. *Energy & Fuels*, 2001. **15**(5): p. 1276-1285.
- 45. Balat, M., Mechanisms of thermochemical biomass conversion processes. Part 2: Reactions of gasification. *Energy Sources Part a-Recovery Utilization and Environmental Effects*, 2008. **30**(7): p. 636-648.
- 46. Gregg, D.W., Aiman, W.R., Otsuki, H.H., and Thorsness, C.B., Solar Coal-Gasification. *Solar Energy*, 1980. **24**(3): p. 313-321.

- 47. Gregg, D.W., Taylor, R.W., Campbell, J.H., Taylor, J.R., and Cotton, A., Solar Gasification of Coal, Activated Carbon, Coke and Coal and Biomass Mixtures. *Solar Energy*, 1980. **25**(4): p. 353-364.
- 48. Taylor, R.W., Berjoan, R., and Coutures, J.P., Solar Gasification of Carbonaceous Materials. *Solar Energy*, 1983. **30**(6): p. 513-525.
- 49. Yu, Q.Z., Brage, C., Chen, G.X., and Sjostrom, K., Temperature impact on the formation of tar from biomass pyrolysis in a free-fall reactor. *Journal of Analytical and Applied Pyrolysis*, 1997. **40-1**: p. 481-489.
- 50. Lichty, P., Perkins, C., Woodruff, B., Bingham, C., and Weimer, A., Rapid High Temperature Solar Thermal Biomass Gasification in a Prototype Cavity Reactor. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(1): p. -.
- 51. Abanades, S., Charvin, P., and Flamant, G., Design and simulation of a solar chemical reactor for the thermal reduction of metal oxides: Case study of zinc oxide dissociation. *Chemical Engineering Science*, 2007. **62**(22): p. 6323-6333.
- 52. Melchior, T., Perkins, C., Weimer, A.W., and Steinfeld, A., A cavity-receiver containing a tubular absorber for high-temperature thermochemical processing using concentrated solar energy. *International Journal of Thermal Sciences*, 2008. **47**(11): p. 1496-1503.
- 53. Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., Hydrogen production from solar thermal dissociation of natural gas: development of a 10 kW solar chemical reactor prototype. *Solar Energy*, 2009. **83**(9): p. 1599-1610.
- 54. Diver, R.B., Miller, J.E., Allendorf, M.D., Siegel, N.P., and Hogan, R.E., Solar thermochemical water-splitting ferrite-cycle heat engines. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2008. **130**(4):.
- 55. Palumbo, R., Keunecke, M., Moller, S., and Steinfeld, A., Reflections on the design of solar thermal chemical reactors: thoughts in transformation. *Energy*, 2004. **29**(5-6): p. 727-744.
- 56. Steinfeld, A. and Fletcher, E.A., A Solar Receiver-Reactor with Specularly Reflecting Walls for High-Temperature Thermoelectrochemical and Thermochemical Processes. *Energy*, 1988. **13**(4): p. 301-311.
- 57. Wieckert, C., Palumbo, R., and Frommherz, U., A two-cavity reactor for solar chemical processes: heat transfer model and application to carbothermic reduction of ZnO. *Energy*, 2004. **29**(5-6): p. 771-787.
- 58. Z'Graggen, A. and Steinfeld, A., Hydrogen production by steam-gasification of carbonaceous materials using concentrated solar energy V. Reactor modeling, optimization, and scale-up. *International Journal of Hydrogen Energy*, 2008. **33**(20): p. 5484-5492.

- 59. Dahl, J.K., Buechler, K.J., Weimer, A.W., Lewandowski, A., and Bingham, C., Solarthermal dissociation of methane in a fluid-wall aerosol flow reactor. *International Journal of Hydrogen Energy*, 2004. **29**(7): p. 725-736.
- 60. Hirsch, D. and Steinfeld, A., Radiative transfer in a solar chemical reactor for the coproduction of hydrogen and carbon by thermal decomposition of methane. *Chemical Engineering Science*, 2004. **59**(24): p. 5771-5778.
- 61. Kogan, A., Israeli, M., and Alcobi, E., Production of hydrogen and carbon by solar thermal methane splitting. IV. Preliminary simulation of a confined tornado flow configuration by computational fluid dynamics. *International Journal of Hydrogen Energy*, 2007. **32**(18): p. 4800-4810.
- 62. Roeb, M., Sattler, C., Kluser, R., Monnerie, N., de Oliveira, L., Konstandopoulos, A.G., Agrafiotis, C., Zaspalis, V.T., Nalbandian, L., Steele, A., and Stobbe, P., Solar hydrogen production by a two-step cycle based on mixed iron oxides. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2006. **128**(2): p. 125-133.
- 63. Moller, S. and Palumbo, R., The development of a solar chemical reactor for the direct thermal dissociation of zinc oxide. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2001. **123**(2): p. 83-90.
- 64. Meier, A., Bonaldi, E., Cella, G.M., Lipinski, W., Wuillemin, D., and Palumbo, R., Design and experimental investigation of a horizontal rotary reactor for the solar thermal production of lime. *Energy*, 2004. **29**(5-6): p. 811-821.
- Kogan, M. and Kogan, A., Production of hydrogen and carbon by solar thermal methane splitting. I. The unseeded reactor. *International Journal of Hydrogen Energy*, 2003. 28(11): p. 1187-1198.
- Hirsch, D. and Steinfeld, A., Solar hydrogen production by thermal decomposition of natural gas using a vortex-flow reactor. *International Journal of Hydrogen Energy*, 2004. 29(1): p. 47-55.
- 67. Schaffner, B., Meier, A., Wuillemin, D., Hoffelner, W., and Steinfeld, A., Recycling of hazardous solid waste material using high-temperature solar process heat. 2. Reactor design and experimentation. *Environmental Science & Technology*, 2003. **37**(1): p. 165-170.
- 68. Piatkowski, N., Wieckert, C., and Steinfeld, A., Experimental investigation of a packedbed solar reactor for the steam-gasification of carbonaceous feedstocks. *Fuel Processing Technology*, 2009. **90**(3): p. 360-366.
- 69. Melchior, T., Perkins, C., Lichty, P., Weimer, A.W., and Steinfeld, A., Solar-driven biochar gasification in a particle-flow reactor. *Chemical Engineering and Processing*, 2009. **48**(8): p. 1279-1287.

- Perkins, C., Lichty, P., Weimer, A.W., and Bingham, C., Fluid-wall effectiveness for preventing oxidation in solar-thermal ZnO reactors. *Aiche Journal*, 2007. 53(7): p. 1830-1844.
- 71. Schunk, L.O., Lipinski, W., and Steinfeld, A., Heat transfer model of a solar receiverreactor for the thermal dissociation of ZnO-Experimental validation at 10 kW and scaleup to 1 MW. *Chemical Engineering Journal*, 2009. **150**(2-3): p. 502-508.
- 72. Maag, G. and Steinfeld, A., Design of a 10 MW Particle-Flow Reactor for Syngas Production by Steam-Gasification of Carbonaceous Feedstock Using Concentrated Solar Energy. *Energy & Fuels*, 2010. **24**: p. 6540-6547.
- 73. Meier, A., Ganz, J., and Steinfeld, A., Modeling of a novel high-temperature solar chemical reactor. *Chemical Engineering Science*, 1996. **51**(11): p. 3181-3186.
- 74. Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., A pilot-scale solar reactor for the production of hydrogen and carbon black from methane splitting. *International Journal of Hydrogen Energy*, 2010. **35**(15): p. 7748-7758.
- 75. Haussener, S., Hirsch, D., Perkins, C., Weimer, A., Lewandowski, A., and Steinfeld, A., Modeling of a Multitube High-Temperature Solar Thermochemical Reactor for Hydrogen Production. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2009. 131(2):.
- 76. Chen, H.J., Chen, Y.T., Hsieh, H.T., and Siegel, N., Computational fluid dynamics modeling of gas-particle flow within a solid-particle solar receiver. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2007. **129**(2): p. 160-170.
- 77. Ozalp, N. and Kanjirakat, A., A Computational Fluid Dynamics Study on the Effect of Carbon Particle Seeding for the Improvement of Solar Reactor Performance. *Journal of Heat Transfer-Transactions of the Asme*, 2010. **132**(12).
- 78. Siegel, N.P., Ho, C.K., Khalsa, S.S., and Kolb, G.J., Development and Evaluation of a Prototype Solid Particle Receiver: On-Sun Testing and Model Validation. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(2): p. -.
- 79. Muller, R., Lipinski, W., and Steinfeld, A., Transient heat transfer in a directly-irradiated solar chemical reactor for the thermal dissociation of ZnO. *Applied Thermal Engineering*, 2008. **28**(5-6): p. 524-531.
- Z'Graggen, A., Haueter, P., Trommer, D., Romero, M., de Jesus, J.C., and Steinfeld, A., Hydrogen production by steam-gasification of petroleum coke using concentrated solar power - II - Reactor design, testing, and modeling. *International Journal of Hydrogen Energy*, 2006. **31**(6): p. 797-811.
- 81. Lipinski, W., Thommen, D., and Steinfeld, A., Unsteady radiative heat transfer within a suspension of ZnO particles undergoing thermal dissociation. *Chemical Engineering Science*, 2006. **61**(21): p. 7029-7035.

- 82. Lipinski, W., Z'Graggen, A., and Steinfeld, A., Transient radiation heat transfer within a nongray nonisothermal absorbing-emitting-scattering suspension of reacting particles undergoing shrinkage. *Numerical Heat Transfer Part B-Fundamentals*, 2005. **47**(5): p. 443-457.
- 83. Maag, G., Lipinski, W., and Steinfeld, A., Particle-gas reacting flow under concentrated solar irradiation. *International Journal of Heat and Mass Transfer*, 2009. **52**(21-22): p. 4997-5004.
- 84. von Zedtwitz, P., Lipinski, W., and Steinfeld, A., Numerical and experimental study of gas-particle radiative heat exchange in a fluidized-bed reactor for steam-gasification of coal. *Chemical Engineering Science*, 2007. **62**(1-2): p. 599-607.
- 85. Klein, H.H., Karni, J., Ben-Zvi, R., and Bertocchi, R., Heat transfer in a directly irradiated solar receiver/reactor for solid-gas reactions. *Solar Energy*, 2007. **81**(10): p. 1227-1239.
- 86. Siegel, R. and Howell, J., *Thermal Radiation Heat Transfer*. 4 ed. 2002, New York: Taylor and Francis.
- 87. Howell, J.R., The Monte Carlo method in radiative heat transfer. *Journal of Heat Transfer-Transactions of the Asme*, 1998. **120**(3): p. 547-560.
- 88. Raithby, G.D. and Chui, E.H., A Finite-Volume Method for Predicting a Radiant-Heat Transfer in Enclosures with Participating Media. *Journal of Heat Transfer-Transactions of the Asme*, 1990. **112**(2): p. 415-423.
- 89. Chui, E.H. and Raithby, G.D., Computation of Radiant-Heat Transfer on a Nonorthogonal Mesh Using the Finite-Volume Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **23**(3): p. 269-288.
- 90. Truelove, J.S., 3-Dimensional Radiation in Absorbing Emitting Scattering Media Using the Discrete-Ordinates Approximation. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1988. **39**(1): p. 27-31.
- 91. Fiveland, W.A., Discrete Ordinate Methods for Radiative Heat-Transfer in Isotropically and Anisotropically Scattering Media. *Journal of Heat Transfer-Transactions of the Asme*, 1987. **109**(3): p. 809-812.
- 92. Z'Graggen, A. and Steinfeld, A., Heat and mass transfer analysis of a suspension of reacting particles subjected to concentrated solar radiation Application to the steam-gasification of carbonaceous materials. *International Journal of Heat and Mass Transfer*, 2009. **52**(1-2): p. 385-395.
- 93. Chai, J.C., Lee, H.S., and Patankar, S.V., Ray Effect and False Scattering in the Discrete Ordinates Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **24**(4): p. 373-389.

- 94. Raithby, G.D., Evaluation of discretization errors in finite-volume radiant heat transfer predictions. *Numerical Heat Transfer Part B-Fundamentals*, 1999. **36**(3): p. 241-264.
- 95. Byun, D.Y., Baek, S.W., and Kim, M.Y., Thermal radiation in a discretely heated irregular geometry using the Monte-Carlo, finite volume, and modified discrete ordinates interpolation method. *Numerical Heat Transfer Part a-Applications*, 2000. **37**(1): p. 1-18.
- 96. Coelho, P.J., The role of ray effects and false scattering on the accuracy of the standard and modified discrete ordinates methods. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2002. **73**(2-5): p. 231-238.
- 97. Sakami, M. and Charette, A., Application of a modified discrete ordinates method to twodimensional enclosures of irregular geometry. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2000. **64**(3): p. 275-298.
- 98. Koo, H.M., Vaillon, R., Goutiere, V., Le Dez, V., Cha, H., and Song, T.H., Comparison of three discrete ordinates methods applied to two-dimensional curved geometries. *International Journal of Thermal Sciences*, 2003. **42**(4): p. 343-359.
- 99. Lathrop, K.D., Ray Effects in Discrete Ordinates Equations. *Nuclear Science and Engineering*, 1968. **32**(3): p. 357-&.
- 100. Baek, S.W., Byun, D.Y., and Kang, S.J., The combined Monte-Carlo and finite-volume method for radiation in a two-dimensional irregular geometry. *International Journal of Heat and Mass Transfer*, 2000. **43**(13): p. 2337-2344.
- 101. Chai, J.C., Hsu, P.F., and Lam, Y.C., Three-dimensional transient radiative transfer modeling using the finite-volume method. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2004. **86**(3): p. 299-313.
- 102. Tan, H.P., Zhang, H.C., and Zhen, B., Estimation of ray effect and false scattering in approximate solution method for thermal radiative transfer equation. *Numerical Heat Transfer Part a-Applications*, 2004. **46**(8): p. 807-829.
- 103. Brown, A.L., Dayton, D.C., and Daily, J.W., A study of cellulose pyrolysis chemistry and global kinetics at high heating rates. *Energy & Fuels*, 2001. **15**(5): p. 1286-1294.
- 104. DiBlasi, C., Heat, momentum and mass transport through a shrinking biomass particle exposed to thermal radiation. *Chemical Engineering Science*, 1996. **51**(7): p. 1121-1132.
- Chan, W.C.R., Kelbon, M., and Kriegerbrockett, B., Single-Particle Biomass Pyrolysis -Correlations of Reaction-Products with Process Conditions. *Industrial & Engineering Chemistry Research*, 1988. 27(12): p. 2261-2275.
- 106. Chan, W.C.R., Kelbon, M., and Krieger, B.B., Modeling and Experimental-Verification of Physical and Chemical Processes during Pyrolysis of a Large Biomass Particle. *Fuel*, 1985. 64(11): p. 1505-1513.

- 107. Bharadwaj, A., Baxter, L.L., and Robinson, A.L., Effects of intraparticle heat and mass transfer on biomass devolatilization: Experimental results and model predictions. *Energy* & *Fuels*, 2004. **18**(4): p. 1021-1031.
- 108. Di Blasi, C., Modeling chemical and physical processes of wood and biomass pyrolysis. *Progress in Energy and Combustion Science*, 2008. **34**(1): p. 47-90.
- 109. Gronli, M.G. and Melaaen, M.C., Mathematical model for wood pyrolysis Comparison of experimental measurements with model predictions. *Energy & Fuels*, 2000. **14**(4): p. 791-800.
- 110. Miller, R.S. and Bellan, J., A generalized biomass pyrolysis model based on superimposed cellulose, hemicellulose and lignin kinetics. *Combustion Science and Technology*, 1997. **126**(1-6): p. 97-137.
- 111. Di Blasi, C., Combustion and gasification rates of lignocellulosic chars. *Progress in Energy and Combustion Science*, 2009. **35**(2): p. 121-140.
- 112. Fushimi, C., Araki, K., Yamaguchi, Y., and Tsutsumi, A., Effect of heating rate on steam gasification of biomass. 1. Reactivity of char. *Industrial & Engineering Chemistry Research*, 2003. **42**(17): p. 3922-3928.
- 113. Wang, Y. and Kinoshita, C.M., Kinetic-Model of Biomass Gasification. *Solar Energy*, 1993. **51**(1): p. 19-25.
- 114. Dupont, C., Boissonnet, G., Seller, J.M., Gauthier, P., and Schweich, D., Study about the kinetic processes of biomass steam gasification. *Fuel*, 2007. **86**(1-2): p. 32-40.
- 115. Papadikis, K., Gu, S., and Bridgwater, A.V., CFD modelling of the fast pyrolysis of biomass in fluidised bed reactors. Part B Heat, momentum and mass transport in bubbling fluidised beds. *Chemical Engineering Science*, 2009. **64**(5): p. 1036-1045.
- 116. Barrio, M., Goble, B., Risnes, H., Henriksen, U., Hustad, J.E., and Sorensen, L.H., *Steam gasification of wood char and the effect oh hydrogen inhibition on the chemical kinetics*, in *Progress in thermochemical biomass conversion*, A. V. Bridgwater, Editor. 2001, Blackwell Science Ltd.: Oxford. p. 32-46.
- 117. Klose, W. and Wolki, M., On the intrinsic reaction rate of biomass char gasification with carbon dioxide and steam. *Fuel*, 2005. **84**(7-8): p. 885-892.
- 118. Harris, D.J. and Smith, I.W., Intrinsic Reactivity of Coke and Char to Carbon-Dioxide. *Abstracts of Papers of the American Chemical Society*, 1989. **197**: p. 44-Fuel.
- 119. Manovic, V., Komatina, M., and Oka, S., Modeling the temperature in coal char particle during fluidized bed combustion. *Fuel*, 2008. **87**(6): p. 905-914.
- 120. Juntgen, H., Reactivities of Carbon to Steam and Hydrogen and Applications to Technical Gasification Processes a Review. *Carbon*, 1981. **19**(3): p. 167-173.

- 121. Laurendeau, N.M., Heterogeneous Kinetics of Coal Char Gasification and Combustion. *Progress in Energy and Combustion Science*, 1978. **4**(4): p. 221-270.
- 122. Muhlen, H.J., Vanheek, K.H., and Juntgen, H., Kinetic-Studies of Steam Gasification of Char in the Presence of H-2, Co2 and Co. *Fuel*, 1985. **64**(7): p. 944-949.
- 123. Muller, R., Von Zedtwitz, P., Wokaun, A., and Steinfeld, A., Kinetic investigation on steam gasification of charcoal under direct high-flux irradiation. *Chemical Engineering Science*, 2003. **58**(22): p. 5111-5119.
- 124. Trommer, D. and Steinfeld, A., Kinetic modeling for the combined pyrolysis and steam gasification of petroleum coke and experimental determination of the rate constants by dynamic thermogravimetry in the 500-1520 K range. *Energy & Fuels*, 2006. **20**(3): p. 1250-1258.
- Long, F.J. and Sykes, K.W., The Mechanism of the Steam-Carbon Reaction. *Proceedings* of the Royal Society of London Series a-Mathematical and Physical Sciences, 1948. 193(1034): p. 377-399.
- 126. Blackwood, J.D. and Mcgrory, F., The Carbon-Steam Reaction at High Pressure. *Australian Journal of Chemistry*, 1958. **11**(1): p. 16-33.
- 127. Maag, G., Rodat, S., Flamant, G., and Steinfeld, A., Heat transfer model and scale-up of an entrained-flow solar reactor for the thermal decomposition of methane. *International Journal of Hydrogen Energy*, 2010. **35**(24): p. 13232-13241.
- 128. Tescari, S., Mazet, N., and Neveu, P., Constructal method to optimize solar thermochemical reactor design. *Solar Energy*, 2010. **84**(9): p. 1555-1566.
- 129. Tescari, S., Mazet, N., Neveu, P., and Abanades, S., Optimization Model for Solar Thermochemical Reactor: Efficiency Increase by a Nonuniform Heat Sink Distribution. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2011. **133**(3).
- 130. Melchior, T. and Steinfeld, A., Radiative transfer within a cylindrical cavity with diffusely/specularly reflecting inner walls containing an array of tubular absorbers. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2008. **130**(2).

## **Chapter II**

# Thermodynamic and practical limitations on receiver efficiency

#### 2.1 Abstract

The maximum efficiency of an open solar receiver/reactor system is limited thermodynamically by the product of the Carnot efficiency and a factor involving both the enthalpy and entropy changes occurring as a result of the chemical reaction. This thermodynamically limiting efficiency can be greater than the Carnot efficiency when the entropy change is positive. Efficiency limitations are evaluated for direct thermolysis of water, steam gasification of carbon or cellulosic biomass, and thermal reduction of ZnO, NiFe<sub>2</sub>O<sub>4</sub>, and Mn<sub>2</sub>O<sub>3</sub>. Inclusion of the entropic and enthalpic terms produces a thermodynamically limiting value of unity under realistic conditions implying that the receiver efficiency for the high temperature step, defined herein as the ratio of the enthalpy change arising from the process occurring in the receiver to the solar energy input, is limited only by the solar energy absorption efficiency. Both the optimal reactor temperature for a given solar concentration ratio, and the solar concentration required to achieve a given temperature and efficiency shift to values lower than those dictated by the Carnot limitation on the system efficiency for the conversion of heat to work. Solar concentration ratios of 3500 and 1575 are required to achieve 70% receiver efficiency for ZnO reduction at 2073 K (1800°C) and NiFe<sub>2</sub>O<sub>4</sub> reduction at 1673 K (1400°C) respectively. These values are well under the corresponding values of 5700 and 3100 identified based on system efficiency.

### **2.2 Introduction**

Concentrated solar energy can be used to reach high temperatures and drive strongly endothermic chemical reactions such as direct water splitting, metal oxide reduction for water splitting cycles, metal oxide carbothermal reduction, and gasification of cellulosic biomass or other carbonaceous materials [1-3]. Species including ZnO, Mn<sub>2</sub>O<sub>3</sub>, Fe<sub>3</sub>O<sub>4</sub>, MFe<sub>2</sub>O<sub>4</sub> (where M is Co, Ni, Mn, or Zn), TiO2, SnO<sub>2</sub>, and CeO<sub>2</sub> have been proposed for metal oxide cycles [2-7]. These cycles couple the strongly endothermic, high temperature thermal reduction of the metal oxide to a lower temperature water oxidation step evolving hydrogen thereby producing hydrogen and oxygen from water in distinct steps. Hydrogen and oxygen can then be recombined in a fuel cell to produce usable work and regenerate water. The complete cycle is shown in Figure 2.1 where the dashed line represents system boundaries if the overall conversion of heat to work is to be considered.



Figure 2.1: System boundaries for the overall conversion of heat to work via a metal oxide water splitting cycle

Many studies detail the thermodynamically-derived efficiency limitations on the overall conversion of solar heat to usable work for water-splitting cycles [1, 2, 8-11]. These studies approach the selection of optimal conditions and solar concentration ratio from the perspective of maximizing the production of work. The system efficiency is defined as the ratio of the work

equivalent of the products to the solar energy input and thus is limited thermodynamically by the Carnot efficiency. In addition to this system efficiency, limitations on the receiver efficiency for the high temperature step alone are of interest for evaluation of solar receiver design and selection of optimum solar concentration or receiver temperature. In this study the solar receiver is approached as an open system and efficiency is defined based on the enthalpy change for the process occurring in the receiver and the solar energy input. The boundaries for this open system are indicated by the dot-dashed line in Figure 2.1. The efficiency defined in this manner is necessarily limited by different values than that based on the work equivalent of the products and use of this definition can have implications on the choice of solar concentration, design of solar fields, and evaluation of process viability.

#### 2.3 Theory

The solar absorption efficiency accounts for physically unavoidable radiative losses through the aperture, while neglecting convective and conductive losses for an idealized receiver, and can be written as in equation 2.1 [1, 2, 8, 12].

$$\eta_{abs} = \frac{\alpha I C - \varepsilon \sigma T^4}{I C} \tag{2.1}$$

Variables  $\alpha$  and  $\varepsilon$  are, respectively, the absorptivity and emissivity of the receiver materials, *I* is the intensity of the incident light, *C* is the concentration ratio over the aperture, and *T* is the receiver temperature. Thermodynamic limitations can be determined by considering a steady state process in which the material entering the reactor (state 1) is transformed into that exiting the reactor (state 2). The boundaries of the process are chosen to include only the solar receiver as shown in Figure 2.2.



Figure 2.2: Schematic boundaries of the solar reaction process

Energy  $Q_h$  is input into the process at a hot temperature  $T_h$ , and energy  $Q_c$  is rejected to the environment at a lower temperature  $T_c$ . The product stream consists of the reaction products, inert gases, and unconverted reactants. Application of the first and second laws of thermodynamics to this system yields equations 2.2 and 2.3 where *H* and *S* are, respectively, the stream enthalpy and entropy.

$$H_1 + Q_h = H_2 + Q_c \tag{2.2}$$

$$S_1 + \frac{Q_h}{T_h} \le S_2 + \frac{Q_c}{T_c} \tag{2.3}$$

Combining equations 2.2 and 2.3 to eliminate  $Q_c$ , and defining the reactor efficiency to be the ratio of the energy required to affect the transformation from state 1 to state 2 to the total energy input, the thermodynamic limitation on the efficiency is given by equation 2.4.

$$\eta_{t} = \frac{\Delta H}{Q_{h}} \le \min \left\{ \frac{\Delta H}{\Delta H - T_{c} \Delta S} \left( 1 - \frac{T_{c}}{T_{h}} \right) \right\}$$
(2.4)

In equation 2.4  $\Delta$  indicates the difference between the outlet and the inlet states, and the limitation of unity arises from the stipulation that the energy rejected to the environment ( $Q_c$ ) is a positive quantity. Here  $\Delta H$  includes both the enthalpy change of reaction and sensible heat requirements. This result is analogous to that presented by both Funk [13, 14] and Pangborn [15]. Equation 2.4 shows that the efficiency of the receiver is not thermodynamically limited

purely by the Carnot efficiency, but by the product of the Carnot efficiency and a coefficient which is strongly dependent on the property changes resulting from the reaction. Note that if the entropy change of the reaction is positive, then the thermodynamic limitation on the receiver efficiency exceeds the Carnot efficiency. The thermodynamically limiting efficiency increases strongly with temperature whereas the absorption efficiency decreases strongly with temperature and increases with the solar concentration ratio. Practically speaking, the receiver efficiency is restricted by the lower of the thermodynamic limitation and the absorption efficiency.

## 2.4 Results

The enthalpic and entropic terms contained within the thermodynamic limitation are computed for various systems including direct thermolysis, reduction of three metal oxides (ZnO, Mn<sub>2</sub>O<sub>3</sub>, and NiFe<sub>2</sub>O<sub>4</sub>), and gasification of carbon or cellulose to carbon monoxide and hydrogen. These terms depend strongly not only on the standard property changes for the reaction, but also on reaction conditions including conversion, temperature, and partial pressures. Table 2.1 shows the calculated values of the coefficient in equation 2.4 for inlet and outlet temperatures equal to the temperature of the external environment (298 K), total inlet and outlet pressures of 1 bar, 100% conversion, and a five to one molar ratio of inert gas to solid reactant.

Reaction	$\frac{\Delta H}{\Delta H - T_c \Delta S}$
$H_2O \rightarrow H_2 + 1/2O_2$	1.22
$ZnO \rightarrow Zn + 1/2O_2$	1.11
$Mn_2O_3 \rightarrow 2MnO + 1/2O_2$	1.24
$NiFe_2O_4 \rightarrow (NiO)(FeO) + 0.5Fe_2O_3 + 0.25O_2$	1.19
$C + H_2 O \rightarrow CO + H_2$	1.82
$C_6H_{10}O_5 + H_2O \rightarrow 6CO + 6H_2$	>5

Table 2.1: Calculated values of the coefficient in equation 2.4

When available, properties are taken from the FactSage thermodynamic databases [16]. Values of the standard entropy or free energy of formation for the cellulose repeat unit are not readily available in the literature and are calculated using thermodynamic data for hydrolysis reactions [17], or estimated from correlations [18, 19]. This leads to a relatively large range of calculated values for the coefficient in equation 2.4; however, for any of these values, the thermodynamically limiting receiver efficiency is unity for the reactor temperatures of interest.

Although each of the values in Table 2.1 at least partially negates the Carnot term in equation 2.4, the coefficient calculated for an outlet temperature of 298 K and 100% conversion is, realistically, an underestimate of the coefficient for more practical reaction conditions. Figure 2.3 illustrates the dependence of the coefficient on the reactor outlet temperature ( $T_2$ ) and the fractional conversion (x) for each for the four chemical reactions given by equations 2.5-2.8 with a total pressure of 1 bar and a five to one molar ratio of argon to solid metal oxide reactant.

$$ZnO \rightarrow xZn + x/2O_2 + (1-x)ZnO$$
(2.5)

$$NiFe_2O_4 \rightarrow (xNiO)(xFeO) + 0.5xFe_2O_3 + 0.25xO_2 + (1-x)NiFe_2O_4$$
 (2.6)

$$C + H_2 O \to C O + H_2 \tag{2.7}$$

$$H_2 O \to x H_2 + x/2 O_2 + (1-x) H_2 O$$
 (2.8)

The coefficient at equilibrium conversion for the outlet temperature is also depicted. The property changes and equilibrium conversions were computed using FactSage software and databases [16] and, for the nickel ferrite reaction, the solutions and species suggested by Allendorf et al. [20]. Sharp variations in the coefficient in Figure 2.3 are due to phase changes in either product or reactant species.



Figure 2.3: Coefficient in equation 2.4 as a function of conversion for (a) ZnO reduction (equation 2.5), (b) NiFe<sub>2</sub>O<sub>4</sub> reduction (equation 2.6) (c) carbon gasification (equation 2.7), (d) water thermolysis (equation 2.8)

Figure 2.4 shows the equilibrium compositions calculated using FactSage as a function of temperature. The coefficient at equilibrium conversion does not always match up directly with the lines for specified conversion because the equilibrium calculation takes into account species not listed in the reactions in equations 2.5-2.8. For instance, the equilibrium mixture for water thermolysis contains  $H_2O$ ,  $H_2$ ,  $O_2$ , H, O, and OH at high temperatures, whereas the specified conversions in Figure 2.3(d) only consider fractional progression of the reaction as written in equation 2.8 without supplementary side reactions.



Figure 2.4: Equilibrium composition with p = 1 bar for (a) ZnO and (b) NiFe<sub>2</sub>O<sub>4</sub> with 5 mol Ar per mol solid reactant, (c) C +H<sub>2</sub>O and (d) H<sub>2</sub>O

At a given reaction temperature  $\Delta H$  increases nearly linearly with conversion whereas  $\Delta S$  increases more slowly due to contributions from the partial pressures of oxygen and inert gas which increase and decrease, respectively, with increasing conversion. This leads to the overall observed increase in the coefficient, and correspondingly  $\eta_t$ , with decreasing conversion. Though not shown in Figure 2.3, when the system contains a large quantity of inert gas, the oxygen generated by the metal oxide reduction reaction is dilute and the partial pressures are nearly independent of conversion. Thus, the coefficient at a given temperature is also nearly independent of conversion. The dashed lines in Figure 2.3 represent the inverse of the Carnot

efficiency assuming the maximum temperature is identical to the outlet temperature. The coefficient in equation 2.4 exceeds the inverse of the Carnot efficiency for any temperature when reaction conversion is either at or below the corresponding equilibrium value.

Figure 2.3 indicates that the thermodynamically limiting efficiency is lowest when the inlet and outlet temperatures are assumed identical. Figure 2.5 shows the absorption efficiency (solid lines) for solar concentration ratios of 500, 1000, 2500, 5000 and 10000 as a function of  $T_h$  along with the minimal thermodynamic limit generated by assuming identical inlet and outlet temperatures for zinc oxide reduction, nickel ferrite reduction, and carbon-steam gasification reactions.



Figure 2.5:  $\eta_{abs}$  (solid lines) and  $\eta_t$  (dashed lines) for (a) ZnO reduction, (b) NiFe<sub>2</sub>O<sub>4</sub> reduction and (c) carbon gasification

Figure 2.5 shows that the minimal thermodynamic limit exceeds the absorption efficiency for all practical reaction conditions. The ZnO thermal reduction typically requires temperatures greater than 2073 K (1800°C) while the NiFe<sub>2</sub>O<sub>4</sub> reduction may be carried out at temperatures greater than 1673 K (1400°C). At these temperatures, the minimal thermodynamically limiting efficiency exceeds the absorption efficiency for all solar concentration ratios below 21,000 and

19,000 for the ZnO and NiFe<sub>2</sub>O<sub>4</sub> reduction reactions, respectively. For a more realistic concentration ratio of 5000, the absorption efficiency is lower than the thermodynamic limit for all temperatures above 1674 K and 1470 K for the ZnO and NiFe<sub>2</sub>O<sub>4</sub> reduction reactions, respectively. Thus practical considerations imposed by unavoidable emission losses provide a more stringent limitation on receiver efficiency than thermodynamic considerations for all realistic ranges of receiver operation.

Figure 2.6 shows the limiting receiver efficiency as a function of the reactor temperature  $(T_h)$  and the concentration ratio. The intensity of the incident light (*I*) is taken to be 1000 W/m<sup>2</sup> and for simplicity  $\alpha = \varepsilon = 1$ . For each of the reactions considered in Figure 2.3 the efficiency of the receiver alone is limited by  $\eta_{abs}$  based on practical considerations with a theoretical thermodynamic limit of unity under realistic conditions. The dashed lines represent the product of the Carnot efficiency and the absorption efficiency, or the efficiency limitation commonly utilized for the conversion of heat to work [2, 8].



Not only is the efficiency of the receiver alone significantly higher than the system efficiency, but the receiver efficiency also decreases monotonically meaning that, for all concentration ratios, the maximum receiver efficiency occurs for the lowest temperature. For a given receiver temperature, a lower solar concentration can be used to attain a desired receiver efficiency than would be needed if the solar concentration ratio was chosen on the basis of system efficiency. For instance, Figure 2.6 shows that for a receiver temperature of 1673 K (1400°C), an efficiency of 70% can be reached with a concentration ratio of approximately C = 1575 (solid lines). However, a concentration ratio of C = 3100 is required to reach a system efficiency of 70% is achieved with a concentration ratio of C = 3500, but a concentration ratio of C = 5700 is required to reach the same system efficiency. Both the higher limiting efficiency at a given temperature or concentration, and the potential for the use of lower concentrations have significant implications on solar field and process design considerations.

### **2.5 Conclusions**

Many studies have determined that the overall conversion of solar heat to usable work for metal oxide water splitting cycles is limited by the Carnot efficiency. However, this limiting value is not directly applicable to the high temperature step alone. The thermodynamic limit on the efficiency of the open receiver system is dependent on enthalpy and entropy changes occurring as a result of the chemical reaction. This limit was assessed for thermal dissociation of H<sub>2</sub>O, steam gasification of carbon or cellulose, and thermal reduction of ZnO, Mn<sub>2</sub>O<sub>3</sub>, and NiFe<sub>2</sub>O<sub>4</sub>. The thermodynamically limiting receiver efficiency was found to exceed the value imposed by emission losses for all reasonable receiver operating conditions. Thus practical considerations imposed by unavoidable emission losses provide a more stringent restriction on receiver efficiency than thermodynamic considerations for all realistic ranges of receiver operation. Selection of receiver operating conditions based on absorption efficiency points

toward the use of lower solar concentration to achieve a given limiting receiver efficiency than would have been identified for an analogous system efficiency.

## Nomenclature

С	concentration ratio at receiver aperture
Н	enthalpy (J mol <sup>-1</sup> )
Ι	solar insolation (W m <sup>-2</sup> )
$Q_c$	heat lost from receiver to environment (W)
$Q_h$	heat input to receiver (W)
S	entropy (J mol <sup>-1</sup> K <sup>-1</sup> )
Т	temperature (K)
x	fractional conversion
α	absorptivity of receiver
З	emissivity of receiver
$\eta_{abs}$	absorption efficiency
$\eta_t$	thermodynamic efficiency
σ	Stefan-Boltzmann constant (W m <sup>-2</sup> K <sup>-4</sup> )

## References

- 1. Fletcher, E.A., Solarthermal processing: A review. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2001. **123**(2): p. 63-74.
- 2. Steinfeld, A., Solar thermochemical production of hydrogen a review. *Solar Energy*, 2005. **78**(5): p. 603-615.
- 3. Kodama, T., High-temperature solar chemistry for converting solar heat to chemical fuels. *Progress in Energy and Combustion Science*, 2003. **29**(6): p. 567-597.
- 4. Sturzenegger, M. and Nuesch, P., Efficiency analysis for a manganese-oxide-based thermochemical cycle. *Energy*, 1999. **24**(11): p. 959-970.
- 5. Nakamura, T., Hydrogen Production from Water Utilizing Solar Heat at High-Temperatures. *Solar Energy*, 1977. **19**(5): p. 467-475.

- 6. Bilgen, E., Ducarroir, M., Foex, M., Sibieude, F., and Trombe, F., Use of Solar-Energy for Direct and 2-Step Water Decomposition Cycles. *International Journal of Hydrogen Energy*, 1977. **2**(3): p. 251-257.
- 7. Abanades, S., Charvin, P., Flamant, G., and Neveu, P., Screening of water-splitting thermochemical cycles potentially attractive for hydrogen production by concentrated solar energy. *Energy*, 2006. **31**(14): p. 2805-2822.
- 8. Fletcher, E.A. and Moen, R.L., Hydrogen and Oxygen from Water. *Science*, 1977. **197**(4308): p. 1050-1056.
- 9. Kodama, T. and Gokon, N., Thermochernical cycles for high-temperature solar hydrogen production. *Chemical Reviews*, 2007. **107**(10): p. 4048-4077.
- 10. Steinfeld, A., Larson, C., Palumbo, R., and Foley, M., Thermodynamic analysis of the co-production of zinc and synthesis gas using solar process heat. *Energy*, 1996. **21**(3): p. 205-222.
- 11. Abraham, B.M. and Schreine.F, General Principles Underlying Chemical Cycles Which Thermally Decompose Water into Elements. *Industrial & Engineering Chemistry Fundamentals*, 1974. **13**(4): p. 305-310.
- 12. Steinfeld, A. and Schubnell, M., Optimum Aperture Size and Operating Temperature of a Solar Cavity-Receiver. *Solar Energy*, 1993. **50**(1): p. 19-25.
- Funk, J.E. and Reinstro.Rm, Energy Requirements in Production of Hydrogen from Water. *Industrial & Engineering Chemistry Process Design and Development*, 1966. 5(3): p. 336.
- 14. Funk, J.E., Thermochemical Processes for Production of Hydrogen from Water. *Abstracts of Papers of the American Chemical Society*, 1976: p. 21-21.
- 15. Pangborn, J.K. and Sharer, J.C., Analysis of Thermochemical Water-Splitting Cycles, in *Proceedings of the Hydrogen Economy Miami Energy Conference (THEME)*, T.N. Veziroglu, Editor. 1975, Plenum Press: Miami, FL. p. 499-515.
- Bale, C., Chartrand, P., Degterov, S.A., Eriksson, G., Hack, K., Ben Mahfoud, R., Melancon, J., Pelton, A.D., and Petersen, S., FactSage thermochemical software and databases. *Calphad-Computer Coupling of Phase Diagrams and Thermochemistry*, 2002. 26(2): p. 189-228.
- 17. Tewari, Y.B. and Goldberg, R.N., Thermodynamics of Hydrolysis of Disaccharides Cellobiose, Gentiobiose, Isomaltose, and Maltose. *Journal of Biological Chemistry*, 1989. **264**(7): p. 3966-3971.
- 18. Prins, M.J., Ptasinski, K.J., and Janssen, F.J.J.G., From coal to biomass gasification: Comparison of thermodynamic efficiency. *Energy*, 2007. **32**(7): p. 1248-1259.

- 19. Szargut, J., Chemical Exergies of the Elements. *Applied Energy*, 1989. **32**(4): p. 269-286.
- 20. Allendorf, M.D., Diver, R.B., Siegel, N.P., and Miller, J.E., Two-Step Water Splitting Using Mixed-Metal Ferrites: Thermodynamic Analysis and Characterization of Synthesized Materials. *Energy & Fuels*, 2008. **22**(6): p. 4115-4124.

## **Chapter III**

# Development of a Monte Carlo model for transport of solar radiation

### **3.1 Introduction**

The inherent complexity of the integro-differential equations governing radiative heat transfer restricts analytical solutions to the simplest scenarios often involving gray-diffuse surfaces and either non-attenuating or isotropically scattering gray media. Consequently, a number of alternative numerical methods have been developed to address physically realistic scenarios involving radiation heat transfer problems. Monte Carlo techniques apply probabilistic models for radiative phenomena and are fully capable of treating absorbing, emitting, anisotropically scattering non-gray media in complex or irregular geometries with spectral or directional optical properties and absorbing or specularly reflective boundary walls [1, 2]. The energy leaving a surface is described by a stochastic number of energy bundles or rays with direction and associated wavelength dictated by physical laws governing radiation exchange. The subsequent sequence of absorption, reflection, or emission events at boundary walls and within a participating media follows the principles governing Markov chains with each event occurring entirely independently from previous events. Monte Carlo methods have been successfully applied for a number of cases including complex enclosures with collimated radiation, bi-directional reflective surfaces, and non-participating media [3-6], calculation of configuration and exchange factors for both diffuse and non-diffuse surfaces with nonparticipating media [7, 8], radiation transport through packed beds [9-11], and radiation transport through absorbing, emitting, anisotropically scattering media [12-15]. Though accurate

treatment of radiative exchange in each of these scenarios is theoretically achievable, excessive computational requirements can arise from the statistical nature of the solutions. Strongly absorbing media are particularly challenging as CPU time increases considerably with the volumetric absorption coefficient of the participating medium [16].

In this study the Monte Carlo technique is applied to transport of solar radiation within the cavity space of a closed-cavity solar receiver filled with a nonparticipating gaseous medium. The solar energy impinging on the exterior window surface is discretized into a large number of rays and the stochastic path of each ray is followed as it travels through the receiver cavity and interacts with various boundary surfaces. Each ray originating at the aperture is followed until it is either absorbed within the receiver or lost by reflection and transmission under the assumption that, once removed, rays cannot re-enter the computational domain. Specular surfaces are presumed to be optically smooth and, as such, spectral directional optical properties are estimated from electromagnetic theory by means of the spectral complex index of refraction describing the material. A diffuse-gray approximation is applied at all strongly absorbing surfaces. The extinction coefficient for quartz is uniformly zero for wavelength between 0.16 -3.6 µm [17] and, as more than 98.5% of the solar spectrum lies within this range, volumetric absorption and emission by the quartz window are ignored. The model detailed herein is generalized to apply to a cylindrical receiver enclosing an array of arbitrarily sized tubes with either an absorbing or reflective cavity surface.

### **3.2 Development of the model**

The direction associated with any ray is identified via the zenith ( $\theta$ ) and azimuth ( $\varphi$ ) angles defined relative to the global coordinate system in Figure 3.1 and calculated from equation 3.1 where  $\hat{i}$ ,  $\hat{j}$ , and  $\hat{k}$  are unit vectors in the *x*, *y*, and *z* directions, respectively.

$$\vec{r} = r_x \hat{i} + r_y \hat{j} + r_z \hat{k} = \sin(\theta) \cos(\phi) \hat{i} + \sin(\theta) \sin(\phi) \hat{j} + \cos(\theta) \hat{k}$$
(3.1)



Figure 3.1: Global coordinate system for the Monte Carlo model

The receiver is situated such that the cavity centroid is placed at the origin of the global coordinate system with the plane representing the window surface described by a uniform positive *x*-coordinate, and tube and cavity wall surfaces extending axially into the vertical *z*-dimension. A three dimensional Monte Carlo model is written for execution in MATLAB<sup>®</sup> and is described by the flow diagram illustrated in Figure 3.2 for solar energy entering through the aperture. A separate incarnation of the model allows for emission of radiative energy from heated surfaces characterized by known temperature profiles. Details of the geometric configuration for the receiver represented schematically in Figure 1.1 are supplied in Figure 3.3 with the window and cooling plate geometry specified in Figure 3.4. Table 3.1 provides equations describing the geometric surfaces comprising the solar receiver along with corresponding surface normal vectors.



Figure 3.2: Flow diagram for a Monte Carlo model describing solar radiation entering through the receiver window



Figure 3.3: Receiver configuration with dimensions in cm



Figure 3.4: Window and cooling plate geometry

Table 3.1. Geometric surfaces and surface normal vectors describing receiver geometry

				Materials	
Surf	face	Surface type, equation	Surface limits	at interface	Surface normal
Tub	oe i	Cylinder $(x - x_{o,i})^2 + (y - y_{o,i})^2 = R_{i,i}^2$	$Z_{cav,min} < Z < Z_{cav,max}$	SiC, Inconel / argon	$n_x = rac{x - x_0}{R_{t,i}}, \ n_y = rac{y - y_0}{R_{t,i}}$ $n_z = 0$
	outer wall	Cylinder $(x)^{2} + (y)^{2} = R_{c}^{2}$	If $x \leq x_{crit} : z_{cav,min} < z < z_{cav,max}$ If $x \geq x_{crit} : z_{cav,min} < z < z_{min}$ $z_{maxl} < z < z_{cav,max}$	Al / argon	$n_x = -\frac{x}{R_c}, \ n_y = -\frac{y}{R_c} \ n_z = 0$
Cavity wall	top	Plane $z = z_{cav,max}$	$egin{aligned} & (x)^2 + (y)^2 \leq R_c^2 \ & (x-x_{o,i})^2 + ig(y-y_{o,i})^2 > R_{t,i}^2 \end{aligned}$	Al / argon	$n_x = n_y = 0$ $n_z = -I$
	bottom	Plane $z = z_{cov,min}$	$(x)^2 + (y)^2 \le R_c^2$ $(x - x_{o,i})^2 + (y - y_{o,i})^2 > R_{t,i}^2$	Al / argon	$n_x = n_y = 0$ $n_z = I$
Window	exterior	Plane $x = x_{wind,surf}$	$y_{minl} < y < y_{maxl}$ and $z_{minl} < z < z_{maxl}$	quartz / argon	$n_y = n_z = 0$ $n_x = I \ (p_{\text{start}} \text{ in exterior})$ $n_x = -I \ (p_{\text{start}} \text{ in window})$
surface	interior	Plane $x = x_{wind,int}$	$y_{minl} < y < y_{maxl}$ and $z_{minl} < z < z_{maxl}$	quartz / argon	$n_y = n_z = 0$ $n_x = I$ (p <sub>start</sub> in window) $n_x = -I$ ( p <sub>start</sub> in cavity )
	top	Plane $x = x_{wind,int}$	$y_{min2} < y < y_{max2}$ $z_{maxl} < z < z_{max2}$	quartz / Al	$n_y = n_z = 0$ $n_x = 1$
Window/	bottom	Plane $x = x_{wind,int}$	$y_{min2} < y < y_{max2}$ $z_{min2} < z < z_{min1}$	quartz / Al	$n_y = n_z = 0$ $n_x = 1$
wall	left	Plane $x = x_{wind,int}$	$y_{min2} < y < y_{min1}$ $z_{min1} < z < z_{max1}$	quartz / Al	$n_y = n_z = 0$ $n_x = 1$
	right	Plane $x = x_{wind,int}$	$y_{maxI} < y < y_{max2}$ $z_{minI} < z < z_{maxI}$	quartz / Al	$n_y = n_z = 0$ $n_x = 1$

Surface normal	$n_x = n_y = 0$ $n_z = -I$	$n_x = n_y = 0$ $n_z = I$	$n_x = n_z = 0$ $n_y = I$	$n_x = n_z = 0$ $n_y = -I$	$n_x = n_y = 0$ $n_z = -1$	$n_x = n_y = 0$ $n_z = I$	$n_x = n_z = 0$ $n_y = I$	$n_x = n_z = 0$ $n_y = -I$	$n_y = n_z = 0$ $n_x = -1$	$n_y = n_z = 0$ $n_x = -1$	$n_y = n_z = 0$ $n_x = -1$	$n_y = n_z = 0$ $n_x = -1$
Materials at interface	Al / argon	Al / argon	Al / argon	Al / argon	quartz / Ni	quartz / Ni	quartz / Ni	quartz / Ni	quartz / Ni	quartz / Ni	quartz / Ni	quartz / Ni
Surface limits	$egin{array}{l} (x)^2 + (y)^2 > R_c^2 \ x_{crit} < x < x_{wind,int} \ y_{mint} < y < y_{maxl} \end{array}$	$(x)^2 + (y)^2 > R_c^2$ $x_{crit} < x < x_{wind,int}$ $y_{mint} < y < y_{maxt}$	$X_{crit} < X < X_{wind,int}$ $Z_{minl} < Z < Z_{maxl}$	$egin{array}{lll} X_{crit} < X < X_{wind,int} \ Z_{minl} < Z < Z_{maxl} \end{array}$	$y_{min2} < y < y_{max2}$ $x_{wind,int} < x < x_{wind,surf}$	$y_{min2} < y < y_{max2}$ $x_{wind,int} < x < x_{wind,surf}$	$Z_{min2} < Z < Z_{max2}$ $X_{wind,int} < X < X_{wind,suf}$	$y_{min2} < y < y_{max2}$ $x_{wind,int} < x < x_{wind,surf}$	$y_{min2} < y < y_{max2}$ $z_{max1} < z < z_{max2}$	$y_{min2} < y < y_{max2}  z_{min2} < z < z_{min1}$	$y_{min2} < y < y_{min1}$ $z_{min1} < z < z_{max1}$	$y_{maxI} < y < y_{max2}$ $z_{minI} < z < z_{maxI}$
Surface type, equation	Plane $z = z_{max_l}$	Plane $z = z_{minl}$	Plane $y = y_{minl}$	Plane $y = y_{maxl}$	Plane $z = z_{max2}$	Plane $z = z_{min2}$	Plane $y = y_{min2}$	Plane $y = y_{max2}$	Plane $x = x_{wind,swf}$	Plane $x = x_{wind,surf}$	Plane $x = x_{wind,swf}$	Plane $x = x_{wind,swf}$
Surface	top	Cavity bottom wall	left	right	top	bottom	left	Window/ right	paner interface top front	bottom front	left front	right front
### 3.2.1 Specification of wavelength

Random values are selected from known probability density functions and cumulative probability distributions through equation 3.2 in which the value of generic variable  $\xi$  is specified by random choice of  $\Re$ .

$$\Re(\xi) = \int_{-\infty}^{\xi} p(\xi^*) d\xi^*$$
(3.2)

The wavelength associated with a given ray is determined randomly in this fashion from Planck's spectral distribution of emissive power  $(e_{\lambda b})$  for a blackbody at temperature *T* in equation 3.3.

$$\Re_{\lambda} = \frac{1}{\sigma T^4} \int_{0}^{\lambda} e_{\lambda b}(\lambda) d\lambda = F_{0-\lambda T}$$
(3.3)

The distribution of wavelengths is fixed by the solar spectrum and approximated as that produced by a blackbody at 5780 K. A table of  $F_{0.\lambda T}$  consisting of 2000 values between 0.1 µm and 12 µm is generated external to the Monte Carlo model for a blackbody temperature of 5780 K in order to minimize the computational expense of calculations carried out within the Monte Carlo model. The wavelength corresponding to the randomly selected  $\Re_{\lambda}$  is determined by interpolation between the values in the table. Additional tables of the spectral complex index of refraction for Al, Ni and quartz are taken from Palik et al. [17] with the value at the randomly selected wavelength calculated by linear interpolation between listed points.

## 3.2.2 Specification of initial ray position

The initial position of any ray is chosen at random from a probability distribution describing the solar flux profile. A uniform flux profile at the receiver window surface can be

specified by equations 3.4 and 3.5 in which  $y_{min1}$ ,  $y_{max1}$ ,  $z_{min1}$ , and  $z_{max1}$  represent the horizontal and vertical extents of the window.

$$\Re_{y} = \frac{y_{initial} - y_{\min 1}}{y_{\max 1} - y_{\min 1}}$$
(3.4)

$$\Re_{z} = \frac{z_{\text{initial}} - z_{\text{min}1}}{z_{\text{max}1} - z_{\text{min}1}}$$
(3.5)

Yet while a uniform profile is beneficial for the purpose of evaluating model solutions under simplified conditions, it is typically an inadequate description of a physically realistic profile. The solar flux at the window surface frequently resembles a Gaussian profile described in equation 3.6 over the range  $y_{min1} \le y \le y_{max1}$  and  $z_{min1} \le z \le z_{max1}$ .

$$F(y,z) = A \exp\left[-\frac{1}{2}\left(\frac{y-y_0}{b}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{z-z_0}{c}\right)^2\right] = AG(y)H(z)$$
(3.6)

The joint probability density function describing solar incidence is equated to the normalized flux profile and, based on the form of equation 3.6, can be recast in terms of two independent probability density functions  $f_y$  and  $f_z$  in equation 3.7.

$$p(y,z) = f_{y}(y)f_{z}(z) = \frac{AG(y)H(z)}{\int_{y_{\min 1}}^{y_{\max 1}} \int_{z_{\min 1}}^{z_{\max 1}} AG(y)H(z)dzdy}$$
(3.7)

As dictated by equation 3.2, initial y and z positions are selected at random from the corresponding independent cumulative distributions functions via equation 3.8 and 3.9 respectively.

$$\Re_{y} = \frac{\int_{y_{\min 1}}^{y} G(y) dy}{\int_{y_{\min 1}}^{y_{\max 1}} G(y) dy} = \frac{erf\left(\frac{y - y_{0}}{b\sqrt{2}}\right) + erf\left(\frac{y_{0} - y_{\min 1}}{b\sqrt{2}}\right)}{erf\left(\frac{y_{\max 1} - y_{0}}{b\sqrt{2}}\right) + erf\left(\frac{y_{0} - y_{\min 1}}{b\sqrt{2}}\right)}$$
(3.8)

$$\Re_{z} = \frac{\int_{z_{\min 1}}^{z} H(z) dz}{\int_{z_{\min 1}}^{z_{\max 1}} H(z) dz} = \frac{erf\left(\frac{z - z_{0}}{c\sqrt{2}}\right) + erf\left(\frac{z_{0} - z_{\min 1}}{c\sqrt{2}}\right)}{erf\left(\frac{z_{\max 1} - z_{0}}{c\sqrt{2}}\right) + erf\left(\frac{z_{0} - z_{\min 1}}{c\sqrt{2}}\right)}$$
(3.9)

The solar receiver described by Figures 1.1, 3.3 and 3.4 is operated on-sun at the High Flux Solar Furnace (HFSF) at the National Renewable Energy Laboratory (NREL). Thus realistic simulations require a solar flux profile analogous to that produced by the HFSF which is shown in Chapter 5 to exhibit complex spatial dependence not adequately described by either a uniform distribution or Gaussian shape. The profile is discussed in detail in Chapter 5 and is evaluated by means of a separate ray tracing routine carried out in the program SolTrace [18] which produces both position and direction for each of roughly 100,000 rays impinging on the window surface. Discrete cumulative probability distributions or discrete cumulative conditional probability distributions for initial ray position and direction are generated from these results as a one-to-one relationship typically does not exist between the SolTrace results and the quantity of rays necessary for a statistically relevant Monte Carlo solution in the receiver cavity. The window is discretized into  $(n_y \ge n_z)$  elements individually denoted by  $e_{ij}$  with constant spacing in both the y and z dimensions for the purpose of generating discrete probability distributions. The probability  $(p_{i,j})$  that a ray will strike element  $e_{ij}$  is given by equation 3.10 where  $N_{i,j}$  is the number of rays incident on window element  $e_{ij}$  from the SolTrace model and the lower y and z boundaries of element  $e_{ij}$  are  $y_i$  and  $z_j$  respectively.

$$p_{i,j} = \frac{N_{i,j}}{\sum_{i=1}^{n_y} \sum_{j=1}^{n_z} N_{i,j}}$$
(3.10)

The matrix of probabilities is converted into a matrix of cumulative probabilities though a summation across elements described by equation 3.11.

$$P_{i,j} = \sum_{k=1}^{i-1} \sum_{m=1}^{n_z} (p_{k,m}) + \sum_{m=1}^{j} p_{i,m}$$
(3.11)

The first term on the right hand side of equation 3.11 is denoted by  $P_{i-1,n_z}$  and represents the cumulative conditional probability for emission in the  $(i-1)^{\text{th}}$  or lower y-division with any z-coordinate. The matrix of cumulative probabilities increases monotonically across each row and is typically defined with  $n_y = n_z = 20$  and generated external to the Monte Carlo model in order to minimize computational requirements. Random selection of initial position proceeds within the Monte Carlo model via random number  $\Re_{pos}$  defined such that a given ray strikes element  $e_{ij}$  if  $\Re_{pos} \leq P_{i,j}$  and  $\Re_{pos} > P_{i,j-1}$ . The continuous (y,z) position of the randomly selected ray is determined in equations 3.12 and 3.13 via additional random numbers  $\Re_y$  and  $\Re_z$  under the assumption of a uniform flux distribution over surface element  $e_{ij}$ .

$$\Re_{y} = \frac{y_{initial} - y_{i}}{y_{i+1} - y_{i}}$$
(3.12)

$$\Re_{z} = \frac{z_{initial} - z_{j}}{z_{j+1} - z_{j}}$$
(3.13)

#### 3.2.3 Specification of initial ray direction

The direction associated with a randomly selected ray at the window surface must also correspond to the profile produced by the HFSF. The window is again discretized into  $(n_y x n_{z_i})$ surface elements with element  $e_{ij}$  defined by minimum y and z coordinates  $y_i$  and  $z_j$  respectively. Both the zenith ( $\theta$ ) and azimuth ( $\varphi$ ) angles are discretized into  $n_{angle}$  uniformly-sized groups. Indices *i* and *j* denote spatial element position on the window surface and are combined into a single index *k* via equation 3.14.

$$k = (i-1)n_z + j \tag{3.14}$$

The conditional probability that a ray incident on window element  $e_k$  has a zenith angle between  $\theta_m$  and  $\theta_{m+1}$  is denoted by  $p^{Z_{k,m}}$  and calculated via equation 3.15 where  $Z_{k,m}$  is the number of rays from the SolTrace model incident on window element  $e_k$  with a zenith angle between  $\theta_m$  and  $\theta_{m+1}$ .

$$p_{k,m}^{Z} = \frac{Z_{k,m}}{\sum_{m=1}^{n_{angle}} Z_{k,m}}$$
(3.15)

The denominator of equation 3.15 represents the total number of rays incident on surface element  $e_k$ . The conditional probability that a ray incident on window element  $e_k$  has a zenith angle less than or equal to  $\theta_{m+1}$  is denoted by  $P^{Z}_{k,m}$  and the corresponding matrix of conditional cumulative probabilities can be assessed from equation 3.16.

$$P_{k,m}^{Z} = \sum_{n=1}^{m} p_{k,m}^{Z} = \frac{\sum_{n=1}^{m} Z_{k,n}}{\sum_{n=1}^{n_{angle}} Z_{k,n}}$$
(3.16)

The conditional cumulative probability matrix  $\mathbf{P}^{\mathbf{Z}}$  is defined such that row *k* represents the cumulative probability distribution describing zenith angle  $\theta$  for window surface element  $e_k$ . Random selection of the surface element  $e_k$  proceeds through the calculations described in section 3.2.2. Random selection of the zenith angle describing the incident ray proceeds within the Monte Carlo model via random number  $\mathfrak{R}_{\theta 1}$  defined such that the zenith angle lies between  $\theta_m$  and  $\theta_{m+1}$  if  $\mathfrak{R}_{\theta 1} \leq P_{k,m}^Z$  and  $\mathfrak{R}_{\theta 1} > P_{k,m-1}^Z$ . The exact value of the initial zenith angle  $\theta_{initial}$  is selected in equation 3.17 by means of a second random number  $\mathfrak{R}_{\theta 2}$  under the assumption of a uniform distribution of angles between  $\theta_m$  and  $\theta_{m+1}$ .

$$\mathfrak{R}_{\theta 2} = \frac{\theta_{initial} - \theta_m}{\theta_{m+1} - \theta_m} \tag{3.17}$$

Distributions of zenith and azimuth angles are not independent and random selection of initial azimuth angle proceeds similarly to the calculations detailed in equations 3.15-3.17. Matrix **A** is defined such that elements  $A_{pq}$  represent the number of rays incident on window element  $e_k = e_{ij}$  with a zenith angle between  $\theta_m$  and  $\theta_{m+1}$  and azimuth angle between  $\varphi_q$  and  $\varphi_{q+1}$ . Matrix **A** has dimensions ( $n_y n_z n_{angle} \times n_{angle}$ ) with row index *p* related to spatial position and zenith angle indices *i*, *j*, and *m* by equation 3.18.

$$p = (i-1)n_z n_{angle} + (j-1)n_{angle} + m$$
(3.18)

The conditional cumulative probability matrix  $\mathbf{P}^{\mathbf{A}}$  is specified in equation 3.19 and defined such that row *p* represents the cumulative probability distribution describing azimuth angle  $\varphi$  for rays striking spatial window surface element  $e_{ij} = e_k$  with a zenith angle between  $\theta_m$  and  $\theta_{m+1}$ .

$$P_{p,q}^{A} = \frac{\sum_{r=1}^{q} A_{p,r}}{\sum_{r=1}^{n_{angle}} A_{p,r}}$$
(3.19)

Random selection of the surface element  $e_k$  proceeds through the calculations described in section 3.2.2 and random selection of the zenith angle range is accomplished through the calculations detailed above. Random selection of the azimuth angle describing the incident ray proceeds within the Monte Carlo model via random number  $\Re_{\varphi_1}$  defined such that the azimuth angle lies between  $\varphi_q$  and  $\varphi_{q+1}$  if  $\Re_{\varphi_1} \leq P_{p,q}^A$  and  $\Re_{\varphi_1} > P_{p,q-1}^A$ . The exact value of the initial azimuth angle  $\varphi_{initial}$  is selected in equation 3.20 by means of a second random number  $\Re_{\varphi_2}$  under the assumption of a uniform distribution of angles between  $\varphi_q$  and  $\varphi_{q+1}$ .

$$\Re_{\varphi^2} = \frac{\varphi_{initial} - \varphi_q}{\varphi_{q+1} - \varphi_q} \tag{3.20}$$

Initial ray vector direction is calculated from the randomly selected zenith and azimuth angles using equation 3.1

A simplified directional input is utilized in limited applications for comparison of Monte Carlo solutions to those obtained by other approximate methods for radiative heat transfer. A diffuse distribution at the aperture is generated by treating each ray as if it were emitted by a diffuse-gray plane at the window surface. The direction is chosen randomly from equation 3.21 and 3.22 where  $e_{Ab}$  is the spectral blackbody emissive power, and  $\alpha$  and  $\beta$  are, respectively, the spherical zenith and azimuth angles defined in relation to the surface normal [2].

$$R(\alpha) = \frac{\int_0^\alpha \int_0^\infty \int_0^{2\pi} e_{\lambda b}(\lambda, \alpha) \sin \alpha d\beta d\lambda d\alpha}{\sigma T^4} = \sin^2 \alpha \qquad (3.21)$$

$$R(\beta) = \frac{\int_0^\beta \int_0^\infty \int_0^{\pi/2} e_{\lambda b}(\lambda, \alpha) \sin \alpha d\alpha d\lambda d\beta}{\sigma T^4} = \frac{\beta}{2\pi}$$
(3.22)

The surface normal coordinate system is described by unit vectors  $\hat{i}'$ ,  $\hat{j}'$ ,  $\hat{k}'$  and defined such that the  $\hat{k}'$  vector is directly aligned with the surface normal. Ray direction is initially specified in the surface normal coordinate system based on random selection of  $\alpha$  and  $\beta$  and then converted to the global coordinate system by means of sequential rotations of the surface normal coordinate axes. The surface normal vector is identified generically by equation 3.23 with the window surface characterized by  $n_y = n_z = 0$ . The vector direction describing the initial ray in the global coordinate system is provided by equation 3.24 with  $n_y = n_z = 0$ .

$$\vec{n}_{s} = n_{x}\hat{i} + n_{y}\hat{j} + n_{z}\hat{k}$$
 (3.23)

$$\vec{r}_{initial} = (n_x \cos \alpha)\hat{i} + (n_x \sin \alpha \cos \beta)\hat{j} + (\sin \alpha \sin \beta)\hat{k}$$
(3.24)

### 3.2.4 Reflection / transmission at external window surface

A given ray originating from the solar concentrating system strikes the external window surface at a position and with a direction  $\vec{r}$  specified in sections 3.2.2 and 3.2.3, respectively. The spectral directional reflectivity of the quartz window surface is calculated from Fresnel's equation for a perfect dielectric [2] as the extinction coefficient of quartz is uniformly zero over 98.5% of the solar spectrum.

$$\rho(\lambda,\delta) = 0.5 \left[ \left( \frac{n_1 \cos \delta - n_2 \cos \delta_{refr}}{n_1 \cos \delta + n_2 \cos \delta_{refr}} \right)^2 + \left( \frac{n_2 \cos \delta - n_1 \cos \delta_{refr}}{n_2 \cos \delta + n_1 \cos \delta_{refr}} \right)^2 \right] \quad (3.25)$$

The refractive index of the medium from which the ray originates is denoted by  $n_1$  whereas  $n_2$  represents the refractive index on the opposing side of the interface. Estimation of surface reflectivity is based on the angle between the surface normal and the incident ( $\delta$ ) or refracted ( $\delta_{refr}$ ) rays defined in Figure 3.5 and calculated by equations 3.26-3.29.



Figure 3.5: Incident, reflected, and refracted ray directions

$$\sin\left(\delta_{refr}\right) = \frac{n_1}{n_2}\sin(\delta) \tag{3.26}$$

$$\cos\left(\delta_{refr}\right) = \left[1 - \sin^2\left(\delta_{refr}\right)\right]^{1/2} \tag{3.27}$$

$$\cos(\delta) = \vec{n}_s \cdot (-\vec{r}) \qquad 0 \le \delta \le \pi/2 \qquad (3.28)$$

$$\sin(\delta) = \left[1 - \cos^2(\delta)\right]^{1/2} \tag{3.29}$$

The incident ray is reflected at the exterior window surface if  $\Re_s \leq \rho(\lambda, \delta)$  and transmitted into the window interior if  $\Re_s > \rho(\lambda, \delta)$ . The calculation is terminated upon reflection of the incident ray under the assumption that the reflected energy cannot re-enter the computational domain. The direction of the transmitted ray is provided in equation 3.30 [2].

$$\vec{r}_{refr} = \frac{n_1}{n_2}\vec{r} + \left(\frac{n_1}{n_2}\cos\delta - \cos\delta_{refr}\right)\vec{n}_s$$
(3.30)

### 3.2.5 Selection of surface interaction

Receiver geometry is specified by means of a set of planar and cylindrical surfaces described in detail in Table 3.1. A generic ray path is characterized by a starting position  $p_{start} = (x_{start}, y_{start}, z_{start})$  and a direction  $\vec{r}$ , both of which are dictated by the position and direction at which the ray left the previous surface interaction. A generic point along the ray path a distance *l* from the starting position is given in equation 3.31 where the (*x*,*y*,*z*) coordinates of point *p* are calculated in equations 3.32-3.34.

$$p = p_{start} + l\vec{r} \tag{3.31}$$

$$x = x_{start} + lr_x \tag{3.32}$$

$$y = y_{start} + lr_y \tag{3.33}$$

$$z = z_{start} + lr_z \tag{3.34}$$

The distance *l* along which the ray must travel prior to intersecting each surface listed in Table 3.1 is calculated provided that such an interaction exists. The value of *l* is determined by combining the equation describing the surface with the equations describing generic point *p*. For planar surfaces, the distance *l* is calculated explicitly from one of equations 3.32-3.34. For cylindrical surfaces, the (*x*,*y*,*z*) coordinates of point *p* are substituted into the equation describing

the cylindrical boundary leading to a quadratic equation with respect to distance *l* as shown in equation 3.35 for a generic cylindrical tube centered at  $(x_0, y_0)$ .

$$(r_x^2 + r_y^2) l^2 + 2 [r_x (x_{start} - x_0) + r_y (y_{start} - y_0)] l + (x_{start} - x_0)^2 + (y_{start} - y_0)^2 - R^2 = 0$$
 (3.35)

The (x,y,z) positions at which the ray impacts each surface are calculated from equations 3.32-3.34 and the prospective interaction is discarded if the (x,y,z) position falls outside of the physical surface boundaries. The ray interacts with the first surface encountered along its path, which can be described by the smallest positive, nonzero value of *l*.

### 3.2.6 Selection of surface reflection / absorption

Any ray striking a given surface may be reflected, absorbed, or transmitted depending on the nature of the surface and corresponding optical properties. Diffuse-gray surfaces produce uniform reflectivity devoid of spectral or directional variability. Spectral directional surface reflectivity for specularly reflecting boundaries is calculated from electromagnetic theory based on the angle ( $\delta$ ) between the surface normal and the incident ray. The surface normal vector is specified generically in equation 3.23 and the component values for each geometric receiver surface are provided in Table 3.1. Directionality of the surface normal vector is chosen such that the vector points into the medium from which an incident ray originates and is defined based on the stipulation in equation 3.36.

$$\vec{n}_{\rm s} \cdot \vec{r} \le 0 \tag{3.36}$$

The angle between the surface normal vector and incident ray is provided by equations 3.28 and 3.29. The reflectivity of an opaque absorbing material characterized by a nonzero extinction coefficient is given by equations 3.37-3.41 for energy originating from a perfect dielectric with an index of refraction of unity [2]. Spectral dependency originates from spectral variability in

the complex index of refraction of the opaque material and this description can be applied at the interface between a gaseous medium and any specular opaque surface in the receiver.

$$\rho(\lambda,\delta) = \left[\rho_{\parallel}(\lambda,\delta) + \rho_{\perp}(\lambda,\delta)\right]$$
(3.37)

$$\rho_{\parallel}(\lambda,\delta) = \frac{a^2 + b^2 - 2a\sin(\delta)\tan(\delta) + \sin^2(\delta)\tan^2(\delta)}{a^2 + b^2 + 2a\sin(\delta)\tan(\delta) + \sin^2(\delta)\tan^2(\delta)}\rho_{\perp}(\lambda,\delta)$$
(3.38)

$$\rho_{\perp}(\lambda,\delta) = \frac{a^2 + b^2 - 2a\cos(\delta) + \cos^2(\delta)}{a^2 + b^2 + 2a\cos(\delta) + \cos^2(\delta)}$$
(3.39)

$$a^{2} = \frac{1}{2} \left\{ \left[ \left( n^{2} - k^{2} - \sin^{2} \delta \right)^{2} + 4n^{2} k^{2} \right]^{1/2} + \left( n^{2} - k^{2} - \sin^{2} \delta \right) \right\}$$
(3.40)

$$b^{2} = \frac{1}{2} \left\{ \left[ \left( n^{2} - k^{2} - \sin^{2} \delta \right)^{2} + 4n^{2}k^{2} \right]^{1/2} - \left( n^{2} - k^{2} - \sin^{2} \delta \right) \right\}$$
(3.41)

The reflectivity at the interface between two perfect dielectrics is given by Fresnel's equation (equation 3.25) which allows for incidence from a medium characterized by an index of refraction greater than unity. All internal and external window surfaces are characterized by this description and incident and refracted directions are specified via equations 3.26 and 3.27 and illustrated in Figure 3.5. Rays which originate from a medium with comparatively higher index of refraction ( $n_1$ ) than that on the opposing side of the interface ( $n_2$ ) may be completely reflected regardless of incident angle provided the incident angle meets the condition given in equation 3.42.

$$\sin(\delta) > \frac{n_2}{n_1} \tag{3.42}$$

Net reflectivity at an interface between semi-transparent and opaque solid media is approximated under the presumption of a small air gap between the solid surfaces in the absence of radiation tunneling and wave interference effects [2]. This description relates to all interfaces at which the quartz window comes into contact with the reflective cavity or cooling plate surfaces and the net reflectivity of the interface is provided by equation 3.43 [2].

$$\rho_{net} = \rho_{SiO2} + \frac{\rho_m (1 - \rho_{SiO2})^2}{1 - \rho_{SiO2} \rho_m}$$
(3.43)

The net reflectivity is higher than that of the individual quartz surface alone ( $\rho_{SiO2}$ ) as a portion of the transmitted energy is reflected by the underlying opaque layer. All radiative energy incident on a quartz/metal interface must, by definition, originate from within the quartz window interior. The reflectivity of the quartz side of the interface ( $\rho_{SiO2}$ ) is calculated from Fresnel's equation accounting for the possibility of total internal reflection, whereas the reflectivity of the metal side of the interface ( $\rho_m$ ) is assessed from equations 3.37-3.41 with  $\delta$  referring to the angle after refraction by the quartz layer. The gap between solid surfaces is presumed small enough that spatial variability arising from multiple reflections at the solid-solid interface may be neglected.

Any ray impinging on a solid surface is reflected if a randomly generated number  $\Re_s$  is less than the surface reflectivity and either absorbed by an opaque surface or transmitted through a semi-transparent boundary if  $\Re_s$  exceeds the surface reflectivity. The direction of a ray transmitted at the interface between two perfect dielectrics is given by equation 3.30 and the direction of a specularly reflected ray is predetermined by the direction of incidence ( $\vec{r}$ ) and described by equation 3.44 [2].

$$\vec{r}_{refl} = \vec{r} - 2(\vec{r} \cdot \vec{n})\vec{n} = \vec{r} + 2\vec{n}\cos\delta$$
(3.44)

Conversely, reflection at a diffuse-gray surface eliminates the directional history of the incident ray and is treated in a manner analogous to emission by a diffuse-gray surface. Diffuse reflection can occur into any direction in the hemisphere above the diffuse surface and the direction of reflection is chosen randomly relative to the surface normal coordinate system by means of equations 3.21 and 3.22 [2] and converted to the global coordinate system by means of sequential rotations of the coordinate axes. Horizontal planar surfaces within the receiver have a surface normal described by  $n_x = n_y = 0$  with  $n_z \neq 0$  and the corresponding direction of the diffusely reflected ray in the global coordinate is given in equation 3.45.

$$\vec{r}_{refl} = (n_z \sin \alpha \cos \beta)\hat{i} + (\sin \alpha \sin \beta)\hat{j} + (n_z \cos \alpha)\hat{k} \quad n_{sx} = n_{sy} = 0$$
(3.45)

Vertical planar and cylindrical surfaces, on the other hand, are characterized by  $n_z = 0$  with  $n_x \neq n_y \neq 0$  and the corresponding direction of the diffusely reflected ray in the global coordinate system is given by equation 3.46.

$$\vec{r}_{refl} = (-n_y \sin\alpha \cos\beta + n_x \cos\alpha)\hat{i} + (n_x \sin\alpha \cos\beta + n_y \cos\alpha)\hat{j} + (\sin\alpha \sin\beta)\hat{k} \quad n_{sz} = 0 \quad (3.46)$$

Both surface reflection and transmission result in a continuation of the calculation. The new starting location and direction of the ray are set to the position of intersection and the corresponding reflected or transmitted direction and the calculation is repeated to determine the location at which the ray next strikes a surface. The process is repeated until the ray is either absorbed or transmitted through the external window surface.

During the calculation, the global position of each surface interaction is retained along with the location at which the ray is eventually absorbed or lost by transmission. Spatial profiles of solar flux either incident on or absorbed by a given surface are generated with surfaces discretized into 10,000-20,000 elements. Once the calculation for each ray is terminated, the global position of each surface interaction is translated into the number of surface interactions occurring within a given surface element. The energy flux either incident on or absorbed by each surface facet is determined from the number of rays incident on or absorbed by the element, the element surface area, and the energy associated with each ray provided by equation 3.47 in

which  $N_{rays}$  is the total number of rays traced during the calculation and  $Q_{solar}$  is the total solar energy impinging on the external window surface

$$e_{ray} = \frac{Q_{solar}}{N_{rays}} \tag{3.47}$$

### 3.2.7 Extension to emission by heated surfaces

Though the Monte Carlo model described above is developed specifically for solar energy introduced through the receiver aperture, minor modifications allow for simulation of energy emitted by heated surfaces with specified surface temperature profiles. Each surface is discretized into individual surface facets with the probability of emission by element *i* calculated in equation 3.48 from the ratio of the energy emitted by element *i* to the total energy emitted by all surfaces.

$$p_{i} = \frac{\varepsilon_{i} \sigma T_{i}^{4} A_{i}}{\sum_{i=1}^{N_{elem}} \varepsilon_{i} \sigma T_{i}^{4} A_{i}}$$
(3.48)

Each element *i* is characterized by surface area  $A_i$ , temperature  $T_i$ , and emissivity  $\varepsilon_i$ . The location at which a ray is emitted is again chosen by means of a randomly generated number  $\Re_{elem}$ . A ray is emitted by element *k* if  $P_{k-1} < \Re_{elem} \le P_k$  where  $P_k$  represents the value of the discrete cumulative probability distribution function given by equation 3.49.

$$P_{k} = \frac{\sum_{i=1}^{k} \varepsilon_{i} \sigma T_{i}^{4} A_{i}}{\sum_{i=1}^{N_{elem}} \varepsilon_{i} \sigma T_{i}^{4} A_{i}}$$
(3.49)

Individual surface facets are prescribed a uniform temperature such that the global position of the emitted ray may be chosen from a uniform distribution over the facet. All emitting surfaces are

assumed diffuse-gray with emission occurring into any direction in the hemisphere above the surface. The emitted direction is chosen randomly in the surface normal coordinate system by means of equations 3.21 and 3.22 then converted to the global coordinate system through sequential rotations of the coordinate axes. The remainder of the calculation proceeds analogously to that described in sections 3.2.5 and 3.2.6 except that the energy associated with each ray is given by equation 3.50.

$$e_{ray} = \frac{\sum_{i=1}^{N_{elom}} \varepsilon_i \sigma T_i^4 A_i}{N_{rays}}$$
(3.50)

## **3.3** Comparison of model results with configuration factors

Results from the Monte Carlo model detailed above are verified for simplistic scenarios involving diffuse-gray boundary surfaces by comparison with numerically and analytically derived values for radiation configuration factors between individual surfaces in the receiver. Though the Monte Carlo model is specified above for the existing receiver geometry, it is written to be valid with variable cavity size and arbitrary size, number and position of tubes. Configuration factors are calculated from the Monte Carlo technique by assuming a uniform temperature distribution for the emitting surface and approximating each surrounding surface as a blackbody so as to computationally eliminate reflection. Initial emitted ray direction in the global coordinate system is chosen at random from equations 3.21, 3.22, 3.45 and 3.46, and configuration factors are assessed from the fraction of rays arriving at the surface of interest.

The radiation configuration factor between the external surface of a diffuse-gray cylinder and an annular disk located at the end of that cylinder was determined by Brockman [19] and can be calculated analytically by equations 3.51 - 3.55.

$$F_{cyl-disk} = \frac{B}{8RH} + \frac{1}{2\pi} \left\{ \cos^{-1}\left(\frac{A}{B}\right) - \frac{1}{2H} \left[\frac{(A+2)^2}{R^2} - 4\right]^{1/2} \cos^{-1}\left(\frac{AR}{B}\right) - \frac{A}{2RH} \sin^{-1}(R) \right\}$$
(3.51)

$$R = \frac{r_{cyl}}{r_{disk}} \tag{3.52}$$

$$H = \frac{h_{cyl}}{r_{disk}} \tag{3.53}$$

$$A = H^2 + R^2 - 1 \tag{3.54}$$

$$B = H^2 - R^2 + 1 \tag{3.55}$$

The cylinder radius and height are, respectively,  $h_{cyl}$  and  $r_{cyl}$ , whereas  $r_{disk}$  is the outer radius of the concentric annular disk located at one end of the cylinder. This spatial arrangement is analogous to a single tube positioned in the center of the receiver and an annular disk representing the top or bottom cavity wall. Table 3.2 displays both the analytical calculations and the minimum and maximum values determined from five iterations of the Monte Carlo calculations as a function of the number of rays. Cylinder height and annular disk radius are 27.9 cm and 9.14 cm respectively whereas cylinder radius varies between 1.27 cm and 2.54 cm. All dimensions are chosen to match those of the existing receiver. The configuration factors generated by Monte Carlo calculations converge toward the analytical solutions as the number of rays increases. The difference between the minimum and maximum values attained through five iterations of the Monte Carlo method with 10<sup>7</sup> rays corresponds to at most 0.3% of the analytical solution.

Configuration factors between a finite rectangle and a finite cylinder of identical length were calculated numerically by Wiebelt and Ruo [20] by means of contour integration. The spatial rectangle/cylinder arrangement geometrically corresponds to the aperture surface and a section of a single tube centered in the cavity with length equivalent to the aperture height.

Analytical calculations						
r <sub>cyl</sub> (cm)	<i>r<sub>cyl</sub> (cm)</i> 1.27		2.54			
$F_{cyl-disk}$	0.089991		0.078443			
	Monte Carlo calculations					
r <sub>cyl</sub> (cm)	r <sub>cyl</sub> (cm) 1.27 2.54					
# rays	Min	Max	Min	Max		
IT Idy5	$F_{cyl-disk}$	$F_{cyl-disk}$	$F_{cyl-disk}$	$F_{cyl-disk}$		
10 <sup>2</sup>	0.05	0.15	0.04	0.12		
$10^{3}$	0.072	0.098	0.062	0.088		
10 <sup>4</sup>	0.0858	0.0915	0.0758	0.0805		
10 <sup>5</sup>	0.08805	0.09154	0.07744	0.07974		
10 <sup>6</sup>	0.089403	0.090299	0.07831	0.078829		
10 <sup>7</sup>	0.0898869	0.0901925	0.07837	0.0785565		

 Table 3.2. Monte Carlo calculations of configuration factors between a cylinder and concentric annular disk compared with analytical solutions

Table 3.3 and 3.4 present, respectively, calculations of the configuration factor for the rectangle to the cylinder ( $F_{rect-cyl}$ ) and for the cylinder to the rectangle ( $F_{cyl-rect}$ ). The cylinder and rectangle heights are identically specified at 9.8 cm with the distance between the cylinder and rectangle centroids set at 9.4 cm. Each dimension is chosen to correspond as closely as possible to those characterizing the existing solar receiver. Wiebelt and Ruo estimated a  $\pm 5\%$  error in each numerically calculated configuration factor. This uncertainty leads to the range of literature values displayed in Table 3.3 for  $r_{cyl} = 1.27$  cm, whereas a slightly higher  $\pm 7.5\%$  error is assumed for the values corresponding to  $r_{cyl} = 2.54$  cm owing to the necessity of linear interpolation between available literature solutions. Configuration factors estimated by the Monte Carlo technique are evaluated directly with emission occurring from either the rectangle surface (Table 3.3) or the cylinder surface (Table 3.4). Literature values for  $F_{cyl} - rect$  in Table 3.4 are determined from the corresponding values of  $F_{rect-cyl}$  in Table 3.3 and the relative surface areas.

Literature values						
r <sub>cyl</sub> (cm)	1.	27	2.54			
Frect-cyl	0.067 - 0.074		0.148 - 0.172			
	Monte Carlo calculations					
$r_{cyl}(cm)$ 1.27		2.54				
# ravs	Min	Max	Min	Max		
# Tays	$F_{rect - cyl}$	$F_{rect - cyl}$	$F_{rect-cyl}$	$F_{rect - cyl}$		
10 <sup>2</sup>	0.05	0.11	0.08	0.19		
10 <sup>3</sup>	0.060	0.093	0.137	0.165		
$10^{4}$	0.0674	0.0733	0.1481	0.1603		
10 <sup>5</sup>	0.06994	0.07379	0.15184	0.15372		
$10^{6}$	0.071057	0.071804	0.154036	0.155007		
10 <sup>7</sup>	0.0714757	0.0715410	0.1541931	0.1542710		

Table 3.3. Monte Carlo calculations for configuration factors between a finite rectangle and finite cylinder of equal length compared with literature values

Table 3.4. Monte Carlo calculations for configuration factors between a finite cylinder and finite rectangle of equal length compared with literature values

Literature values					
r <sub>cyl</sub> (cm)	1.1	27	2.	2.54	
$F_{cyl-rect}$	0.048 - 0.053		0.053 - 0.062		
Monte Carlo calculations					
r <sub>cyl</sub> (cm)	1.27 2.54			54	
# rays	Min	Max	Min	Max	
# 1ays	$F_{cyl-rect}$	$F_{cyl}$ - rect	$F_{cyl-rect}$	$F_{cyl}$ - rect	
10 <sup>2</sup>	0.03	0.08	0.03	0.09	
10 <sup>3</sup>	0.043	0.063	0.041	0.072	
$10^{4}$	0.0487	0.0552	0.0518	0.0586	
10 <sup>5</sup>	0.04997	0.05241	0.05422	0.05681	
10 <sup>6</sup>	0.050918	0.051625	0.054965	0.055482	
10 <sup>7</sup>	0.0510847	0.0512701	0.0551213	0.0552677	

The configuration factors generated by Monte Carlo calculations converge toward the range of literature values as the number of rays increases. Results in Tables 3.2-3.4 signify that at least  $10^4 - 10^5$  rays are required for configuration factors accurate to a single significant figure whereas configuration factors accurate to two significant figures require  $10^6 - 10^7$  rays.

## **3.4 Conclusions**

A Monte Carlo model was developed to approximate radiative transfer within a nonparticipating medium in the cavity space of a closed cavity solar receiver. Though the Monte Carlo model was specified for the existing receiver geometry, it was written such that its validity extends to any cylindrical cavity receiver enclosing an arbitrary array of tubular surfaces. Surfaces may be either diffuse-gray or specularly reflective with spectral directional optical properties of optically smooth specular surfaces determined via electromagnetic theory as a function of the complex index of refraction of the material. The model was intended for the approximation of solar radiative energy introduced at the aperture and, as such, volumetric absorption within the quartz window was ignored as the extinction coefficient is negligible over a spectral range encompassing more than 98% of the solar energy. Random selection of initial ray position and vector direction at the aperture arose from a variety of continuous or discrete probability distributions. A separate incarnation of the model was applied to energy diffusely emitted by heated surfaces with specified temperature profiles.

Solutions from the Monte Carlo model were verified for simplistic scenarios by comparison with numerically and analytically derived literature values for radiation configuration factors between individual surfaces in the receiver. Monte Carlo solutions converged toward the numerical or analytical literature values as the number of rays increased and configuration factors accurate to within at least two significant figures required 10<sup>7</sup> rays. Validation of the Monte Carlo solutions for more realistically complex scenarios involving directionally-dependent energy distributions and specularly reflective surfaces with spectral directional optical properties is more challenging as analytical solutions are not readily available in the literature. Monte Carlo solutions will be compared to calculations from an alternate class of approximate techniques for geometric configurations and conditions characteristic of solar receivers in the subsequent chapter.

## Nomenclature

A	surface area
$A_{p,q}$	number of rays incident on window element k with zenith angle between $\theta_m$ and
	$\theta_{m+1}$ and azimuth angle between $\varphi_q$ and $\varphi_{q+1}$
$e_{\lambda b}$	spectral emissive power
<i>e</i> <sub>ray</sub>	energy associated with single ray
$F_{0-\lambda T}$	blackbody fraction
F <sub>i-j</sub>	configuration factor between surfaces i and j
$h_{cyl}$	cylinder height for configuration factor calculations
k	extinction coefficient
l	distance
n	refractive index
n <sub>angle</sub>	number of divisions in each zenith and azimuth angles for discrete ray
	probability distributions
$n_y$	number of divisions of window surface in y-dimension for flux profile
	specification
$n_z$	number of divisions of window surface in z-dimension for flux profile
	specification
$\vec{n}_s$	surface normal vector
$N_{i,j}$	number of rays on window element i,j

N <sub>rays</sub>	number of rays
Nelem	number of surface elements
<i>p</i> <sub>start</sub>	starting point for ray
р	probability distribution
Р	cumulative probability distribution
$Q_{solar}$	total solar power
$\vec{r}$	ray direction vector
<i>r<sub>cyl</sub></i>	cylinder radius for configuration factor calculations
<i>r</i> <sub>disk</sub>	annular disk outer radius for configuration factor calculations
R	radius
R	random number
Т	temperature
$Z_{k,m}$	number of rays incident on window element k with zenith angle between
	$\theta_m$ and $\theta_{m+1}$
α	zenith angle in surface normal coordinate system
β	azimuth angle in surface normal coordinate system
$\delta$	angle between incident ray and surface normal
З	surface emissivity
$\theta$	zenith angle in global coordinate system
λ	wavelength
ρ	surface reflectivity
$\rho_{net}$	total reflectivity of semi-transparent/opaque material interface
σ	Stefan-Boltzmann constant
arphi	azimuth angle in global coordinate system

# Subscripts and superscripts

A	azimuth angle
b	blackbody
С	cavity
0	initial or center
t	tube

refl	reflected
refr	refracted
x	component of vector in x direction
У	component of vector in y direction
Ζ	component of vector in z direction
Ζ	zenith angle
λ	wavelength
1	medium on incidence side of semi-transparent interface
2	medium on transmitted side of semi-transparent interface
	polarized parallel to incident plane
$\perp$	polarized perpendicular to incident plane

## References

- 1. Howell, J.R., The Monte Carlo method in radiative heat transfer. *Journal of Heat Transfer-Transactions of the Asme*, 1998. **120**(3): p. 547-560.
- 2. Siegel, R. and Howell, J., *Thermal Radiation Heat Transfer*. 4 ed. 2002, New York: Taylor and Francis.
- 3. Corlett, R.C., Direct Monte Carlo Calculation of Radiative Heat Transfer in Vacuum. *Journal of Heat Transfer*, 1966. **88**(4): p. 376.
- 4. Howell, J.R. and Durkee, R.E., Radiative Transfer between Surfaces in a Cavity with Collimated Incident Radiation Comparison of Analysis and Experiment. *Journal of Heat Transfer*, 1971. **93**(2): p. 129.
- 5. Maltby, J.D. and Burns, P.J., Performance, Accuracy, and Convergence in a 3-Dimensional Monte-Carlo Radiative Heat-Transfer Simulation. *Numerical Heat Transfer Part B-Fundamentals*, 1991. **19**(2): p. 191-209.
- 6. Toor, J.S. and Viskanta, R., A Numerical Experiment of Radiant Heat Interchange by Monte Carlo Method. *International Journal of Heat and Mass Transfer*, 1968. **11**(5): p. 883.
- 7. Yarbrough, D. and C., L., *Monte Carlo Calculation of Radiation View Factors*, in *Integral Methods in Science and Engineering*, F. Payne, Editor. 1986, Hemisphere: Washington, DC. p. 563-574.

- 8. Modest, M.F., Three-Dimensional Radiative Exchnag Factors for Nongray Nondiffuse Surfaces. *Numerical Heat Transfer Part B-Fundamentals*, 1978. **1**(3): p. 403-416.
- 9. Yang, Y.S., Howell, J.R., and Klein, D.E., Radiative Heat-Transfer through a Randomly Packed-Bed of Spheres by the Monte-Carlo Method. *Journal of Heat Transfer-Transactions of the Asme*, 1983. **105**(2): p. 325-332.
- Singh, B.P. and Kaviany, M., Independent Theory Versus Direct Simulation of Radiation Heat-Transfer in Packed-Beds. *International Journal of Heat and Mass Transfer*, 1991. 34(11): p. 2869-2882.
- 11. Singh, B.P. and Kaviany, M., Modeling Radiative Heat-Transfer in Packed-Beds. *International Journal of Heat and Mass Transfer*, 1992. **35**(6): p. 1397-1405.
- 12. Farmer, J.T. and Howell, J.R., Monte-Carlo Prediction of Radiative Heat-Transfer in Inhomogeneous, Anisotropic, Nongray Media. *Journal of Thermophysics and Heat Transfer*, 1994. **8**(1): p. 133-139.
- 13. House, L.L. and Avery, L.W., Monte Carlo Technique Applied to Radiative Transfer. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1969. **9**(12): p. 1579.
- 14. Howell, J.R. and Perlmutter, M., Monte-Carlo Solution of Radiant Heat Transfer in a Nongrey Nonisothermal Gas with Temperature Dependent Properties. *Aiche Journal*, 1964. **10**(4): p. 562-567.
- Taniguchi, H., Kudo, K., Otaka, M., Sumarsono, M., and Obata, M., Development of a Monte-Carlo Method for Numerical-Analysis on Radiative Energy-Transfer through Nongrey-Gas Layer. *International Journal for Numerical Methods in Engineering*, 1992. 35(4): p. 883-891.
- 16. Surzhikov, S.T. and Howell, J.R., Monte Carlo simulation of radiation in scattering volumes with line structure. *Journal of Thermophysics and Heat Transfer*, 1998. **12**(2): p. 278-281.
- 17. Palik, E.D., ed. *Handbook of Optical Constants of Solids*. 1998, Academic Press: San Diego.
- 18. Wendelin, T. SolTRACE: A new optical modeling tool for concentrating solar optics. in *Proceedings of the ISEC: International Solar Energy Conference*. 2003. Kohala Coast, Hawaii: American Society of Mechanical Engineers.
- 19. Brockmann, H., Analytic angle factors for the radiant interchange among the surface elements of two concetnric cylinders. *International Journal of Heat and Mass Transfer*, 1994. **37**(7): p. 1095-1100.
- 20. Wiebelt, J.A and Ruo, S.Y., Radiant-interchange configuration factors for finite right circular cylinder to rectangular plane. *International Journal of Heat and Mass Transfer*, 1963. **6**(2): p. 143-146.

## **Chapter IV**

# Evaluation of finite volume solutions for thermal radiative heat transfer in a closed cavity solar receiver for high temperature solar thermal processes

## 4.1 Abstract

High temperature solar-thermal reaction processes can be carried out within closed-cavity solar receivers in which concentrated solar energy enters the cavity through a small aperture or window and is absorbed either directly by reactants or by tubes containing reactant mixtures. Accurate modeling of radiation transfer phenomena in the solar receiver is critical for predicting receiver performance and improving receiver design. Finite volume based radiation heat transfer models are subject to both false scattering and ray concentration errors, and the interaction between these errors can produce unexpected results. The accuracy of the finite volume (FV) method is evaluated in comparison to Monte Carlo (MC) techniques for both the concentrated solar energy and the energy emitted by heated surfaces in a receiver with either absorbing and diffusely emitting or specularly reflective cavity walls. Models are solved for two-dimensional slices of each of two receiver configurations with four spatial grids ranging from 2,300 to 133,000 mesh elements, and three different angular grids. Solar radiative energy is described by a simplified uniform spatial profile at the receiver aperture that is either collimated, diffuse, or contained within a 30 degree cone. Quantitatively accurate FV solutions for the solar energy either require highly refined angular and spatial grids, or are not possible on the mesh sizes investigated in this study whereas FV solutions for the emitted energy are sufficient even on coarse angular and spatial grids. FV solutions are least accurate when the cavity is highly

specularly reflective or the absorber area is minimized, and tend to improve as the character of the incident solar energy changes from collimated to diffuse. Based on these results, a hybrid Monte Carlo/finite volume strategy is proposed for use in combined radiation and convection/conduction heat transfer models.

## **4.2 Introduction**

Computational models are frequently used to predict temperature and corresponding reactant conversion or solar-to-chemical efficiency for closed cavity solar receivers utilized to carry out thermochemical processes driven by solar energy. Concentrated solar energy typically constitutes the only external heat source and, correspondingly, performance of the overall receiver heat transfer model is closely tied to the accuracy of the radiation model. Finite volume or discrete ordinates [1-4], radiosity [5-7], and Monte Carlo [8-11] methods are commonly employed to solve the radiative heat transfer problem. The finite volume (FV) [12, 13] and discrete ordinates (DO) [14, 15] methods for radiative transfer are appealing as they are capable of treating non-isothermal, absorbing, emitting, anisotropically scattering, non-gray media in complex geometries while retaining compatibility with a control volume based computational fluid dynamics modeling approach leading to close coupling between solutions for radiative energy and detailed surface temperature profiles [12]. However, previous studies have detailed various maladies, namely ray effects and false scattering errors, that afflict the solutions of finite volume based methods and whose effects can be both problematic and difficult to eliminate [16, 17]. Ray effects originate from the approximation of a continuum angular distribution with a finite set of directions and can never be completely eliminated from finite volume solutions. False scattering, on the other hand, arises from approximation of intensity values at control

volume faces from surrounding nodal values and produces a general smearing of the intensity field.

A number of studies have investigated the accuracy of variations of the DO and FV methods in enclosures with partially heated surfaces, diffuse-gray walls, and diffuse or collimated incident radiative energy [16-24]. In enclosures with partially heated walls, ray effects are most pronounced for a localized or isolated heat source and worsen as the heated length [18, 19, 21, 23] and the optical thickness [16, 18, 19] of the medium decreases or as the surface reflectivity increases [22]. Many authors have noted that ray effects and false scattering produce opposing errors such that solution oscillations due to ray effects are artificially smoothed by false scattering [16, 17, 20, 21, 25]. Therefore independently improving either the spatial or angular discretization does not necessarily result in a superior solution and relatively accurate solutions may be obtained on coarse angular and spatial grids despite individually large ray effect and false scattering errors. As spatial discretization alone is improved, false scattering is minimized and fails to compensate for ray effect errors potentially leading to less accurate solutions.

Solutions obtained via Monte Carlo (MC) methods are not subject to discretization errors and are typically used to obtain benchmark values [26, 27]. MC methods apply probabilistic models for radiative exchange and, though highly accurate within a statistical limit, are not directly compatible with control-volume based computational fluid dynamics (CFD) approaches. The aim of this study is to examine the accuracy of the finite volume (FV) method for two closed-cavity solar receiver configurations in order to assess the feasibility of using the FV method to solve the radiative transfer equation within an overall CFD simulation of the solar receiver. While many past studies quantifying errors in FV and DO solutions have been carried out for gray enclosures with absorbing/emitting/scattering media and diffusely emitted radiation, relatively few have been performed for highly specularly reflective enclosures with the collimated or strongly directionally-dependent intensity distributions that typically result from solar concentrating facilities.

## 4.3 Radiation models

Cross sections of two cavity receiver configurations are depicted in Figure 4.1. Both designs consist of a circular cavity enclosure and a flat aperture surface. One configuration has five staggered tubes enclosed in a circular cavity with dimensions identical to a cross section of the receiver described by Lichty et al. [28] illustrated in Figures 1.1 and 3.3. The second configuration has an identical cavity design with a centered single tube. The single tube geometry is included to provide a more stringent test of the finite volume method as the placement of the tube maximizes cavity wall reflections.



Figure 4.1: Receiver configurations with dimensions in cm for (a) one centered tube and (b) five staggered tubes

For simplicity the cavity medium is assumed to be non-participating and only uniform optical properties are considered. In all cases the tubes are assumed diffuse with an absorptivity of 0.96.

The cavity walls are treated as either specularly reflective with a uniform reflectivity of 0.9 or diffuse-gray with a uniform reflectivity of 0.1 to represent the use of realistic reflective or absorbing cavity materials. The radiative energy originating from the solar concentrating system and incident on the receiver aperture is, for simplicity, assumed uniform across the aperture and stipulated to be either collimated, diffuse, or evenly distributed within a 30° cone centered around the angle perpendicular to the aperture. Solar energy is assessed separately from that emitted by heated receiver surfaces in order to evaluate FV method accuracy individually for each component.

### 4.3.1 Finite Volume (FV) Method

The finite volume method has been described frequently in the literature [12, 13] and only a brief description is repeated here. The radiative transfer equation describes the radiation intensity at any position along a path in an absorbing, emitting and scattering medium and is written in equation 4.1.

$$\frac{dI(r,s)}{ds} = -(a+\sigma_s)I(r,s) + aI_b(r) + \frac{\sigma_s}{4\pi} \int_0^{4\pi} I(r,s')\Phi(s,s')d\omega'$$
(4.1)

The finite volume scheme is implemented in the commercial software ANSYS FLUENT version 6.3.26 which employs the finite volume method of Chui and Raithby and its extension to unstructured meshes [12, 13, 29]. Each octant of space is divided into  $(N_{\theta} \times N_{\phi})$  control angles with constant  $\theta$  and  $\phi$  extents leading to  $8N_{\theta}N_{\phi}$  total control angles in three-dimensional simulations and  $4N_{\theta}N_{\phi}$  in two-dimensional simulations due to symmetry. The finite volume method integrates equation 4.1 over each control volume and solid angle  $\omega^{l}$  with intensity taken as uniform over each solid angle. Only non-participating media are considered in this study, thus the integrated radiative transfer equation becomes, with no solid angle overhang:

$$\sum_{f=1}^{N_f} A_{s,f} I_{if}^{\ell} \vec{n}_f \cdot \int_{\omega^{\ell}} \vec{s} d\omega = 0$$

$$(4.2)$$

When control angle boundaries are not aligned with mesh faces the intensity is subdivided into incoming and outgoing intensities through the use of pixelization [29]. Each control angle is divided into  $(N_{\theta p} x N_{\Phi p})$  auxiliary solid angles and the analogous form of equation 4.2 is:

$$\sum_{f=1}^{N_f} A_{s,f} \left( I_{if,out}^{\ell} \vec{n}_f \cdot \sum_{\vec{s}^{p\ell} \cdot \vec{n}_f > 0} \int_{\omega^{p\ell}} \vec{s} d\omega + I_{if,in}^{\ell} \vec{n}_f \cdot \sum_{\vec{s}^{p\ell} \cdot \vec{n}_f < 0} \int_{\omega^{p\ell}} \vec{s} d\omega \right) = 0$$

$$(4.3)$$

The integrals in equation 4.3 are carried out over the pixel solid angles and are purely geometric factors. The interior summations are carried out over all pixels within a control angle and directions  $\vec{s}^{p\ell}$  represent the direction of the pixel solid angle centroids. In this study a second order upwind discretization scheme is employed and the face values are computed from the nodal value and the gradient in the upwind control volume. All gradients are approximated using a Green-Gauss node-based evaluation.

The outgoing intensity at solid walls is provided by either equation 4.4 for diffusely emitting and reflecting boundaries, or by equation 4.5 for diffusely emitting and specularly reflecting boundaries.

$$I(r_w,\vec{s}) = \frac{\varepsilon_w \sigma T_w^4}{\pi} + \frac{\rho_w}{\pi} \int_{\vec{s}' \cdot n_w < 0} I(r_w,\vec{s}') |\vec{s} \cdot \vec{n}_w| d\omega$$
(4.4)

$$I(r_w, \vec{s}) = \frac{\varepsilon_w \sigma T_w^4}{\pi} + \rho_w I(r_w, \vec{s}')$$
(4.5)

The reflected and incident directions in equation 4.5 are denoted by  $\vec{s}$  and  $\vec{s}'$  respectively and related in equation 4.6.

$$\vec{s}' = \vec{s} - 2(\vec{s} \cdot \vec{n}_w)\vec{n}_w \tag{4.6}$$

### 4.3.2 Monte Carlo (MC) method

Finite volume solution accuracy is evaluated in comparison with solutions obtained from the Monte Carlo (MC) method. Only an outline of the method is presented here, details can be found in Chapter 3. The MC method follows a large number of bundles of energy as each travels through the enclosure and interacts with boundary surfaces. In this study only a non-attenuating cavity medium is considered and transport of solar radiation is evaluated independently from transport of radiation emitted by heated surfaces in the receiver. Initial positions and directions of rays are determined randomly from the corresponding probability density functions. For the solar component, all radiation originates from the plane describing the aperture surface and the initial direction is determined from a prescribed distribution. The initial positions of emitted rays are determined at random from a matrix of probabilities derived from the temperature distribution of each surface element, and emitted directions correspond to a diffuse distribution. Upon interaction with an enclosure surface, each ray is absorbed, transmitted, or reflected based on a random choice. For diffuse surfaces, the direction of reflection is determined randomly whereas for specular surfaces the direction of reflection is specified by the direction of incidence. The calculation is terminated when each ray is either absorbed or lost by transmission out of the transparent window surface. All surfaces are subdivided into individual elements with the energy flux incident on each element computed from the element area and the number of incident rays.

## 4.4 Results and Discussion

All Monte Carlo solutions are obtained with  $10^7$  rays and the solar energy flux profiles are normalized to the solar flux incident on the receiver window. The absorption efficiency,  $\eta_{abs}$ , is computed from the integral of the normalized absorbed surface heat flux ( $q_{abs,n}$ ). Table 4.1 displays the maximum difference in  $q_{abs,n}$  and  $\eta_{abs}$  between repeated simulations as a function of the number of rays for the five tube geometry with either collimated or diffuse incident solar radiation and a reflective cavity. The spatial profile at the aperture is presumed uniform for simplicity. Results for the single tube geometry are similar. Large discrepancies present in the MC heat flux solutions with a small number of rays decrease to less than 1% of the normalized solar energy flux incident on the receiver aperture for 10<sup>7</sup> rays. Maximum errors in the absorption efficiency for any surface are at most 0.46% of the total solar energy incident on the aperture even with a small number of rays. These values represent errors as high as 40% of the solar energy absorbed by the given surface for 10<sup>4</sup> rays and decrease to 0.4% for 10<sup>7</sup> rays.

	# rays	$Max(q_{abs,n,1})$	$-q_{abs,n,2}\Big)$	$Max(\eta_{abs,1}$	$-\eta_{abs,2} )$
		Collimated	Diffuse	Collimated	Diffuse
	$10^{4}$	0.24	0.15	0.0046	0.0033
	10 <sup>5</sup>	0.072	0.042	0.0040	0.0014
	10 <sup>6</sup>	0.036	0.020	0.0011	0.0007
	$10^{7}$	0.009	0.005	0.00032	0.00025

Table 4.1: Maximum error in normalized surface heat flux and absorption efficiency

FV method solutions are carried out in half of the two-dimensional slices depicted in Figure 4.1 by taking advantage of the symmetry of the center line. The FV method is solved on each of four different unstructured grids with 2364, 23186, 83700, and 133002 mesh elements for the single tube configuration or 3130, 23550, 80789 and 132453 elements for the five tube configuration. Spatial mesh is generated for each design based on identical interval spacing as a fraction of total edge length. Control angles are specified with ( $N_{\theta} x N_{\phi}$ ) = (5x5), (15x15), and (25x25) and pixelization is maintained at (3 x 3).

Table 4.2 provides approximate solution times for the FV method on a single core of an Intel Core 2 Duo Quad CPU for the five tube configuration with collimated solar radiation. Solution time increases dramatically as the number of control angles and mesh elements increases. Table 4.3 provides approximate MC method solution times on a single Pentium D CPU. Cavity reflections are most prevalent in reflective cavity and single tube configurations and lengthen the solution time by increasing the number of surface interactions occurring prior to absorption or transmission of each ray. While the values in Tables 4.2 and 4.3 are not directly comparable it can be estimated that the MC model is similar in computational intensity to the 2D FV models with the highest angular and spatial grid refinement.

 Table 4.2: Approximate solution time (s) for the 2D FV method for the five tube configuration with collimated solar radiation

Mesh	$N_{\theta} = N_{\Phi}$			
elements	5	15	25	
3130	11	97	270	
23550	140	770	2100	
80789	570	4200	12000	
132453	1000	8800	20000	

Table 4.3: Approximate solution time (s) for the 2D MC method with  $10^7$  rays

Solar	Geometry	Cavity	
radiation		Reflective	Absorbing
Collimated	1 tube	25900	11400
Diffuse	1 tube	29400	11800
Collimated	5 tube	11500	12000
Diffuse	5 tube	20300	12400

Results from the FV method based on 133022 or 132453 spatial mesh elements are nearly identical to those based on 83700 or 80789 spatial mesh elements regardless of angular grids

specification and are not shown in the subsequent figures. Similarly, refining the angular grid from  $(N_{\theta} \times N_{\phi}) = (15 \times 15)$  to  $(25 \times 25)$  only produced marginal improvements in solution accuracy and thus the  $(25 \times 25)$  angular grid is omitted for brevity.

### 4.4.1 Collimated incident solar radiation

Figures 4.2 and 4.3 show profiles of the normalized radiative energy flux incident on the tube and cavity walls for the single tube configuration when the solar radiation is treated as a uniform collimated beam originating from the receiver aperture.



Figure 4.2: Profiles of normalized collimated solar energy flux incident on the single tube surface for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (c)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity; (d)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

All flux values are normalized to the uniform radiative flux incident on the receiver aperture and the angle  $\beta$  is measured around the tube circumference counterclockwise from the direction facing toward the aperture. The tube is positioned at the center of the circular cavity and, consequently, it is physically impossible for energy which misses the tube on the first pass to strike the tube after any number of specular cavity reflections. However, the slight non-zero diffuse reflectivity of the tube walls provides a mechanism by which a small amount of energy may impinge on the back of the tube. Thus the MC solutions in Figure 4.2 are clearly dominated by direct incidence and are nearly indistinguishable for absorbing and reflective cases. FV solutions for the reflective case exhibit a substantial quantity of solar energy incident on the back of the tube implying that some portion of the radiation reflected by the cavity walls eventually reaches the tube in the numerical calculation. The results for the reflective case with  $(N_{\theta} \times N_{\phi}) = (5x5)$  do not improve as the number of spatial mesh elements increases suggesting that ray effect errors dominate the solution on the coarse angular grid. These errors decrease when  $(N_{\theta} x N_{\phi}) = (15x15)$ , but discrepancies remain large even with  $(N_{\theta} x N_{\phi}) = (25x25)$  and 133002 mesh elements. Comparatively, FV solutions for the absorbing case are reasonably accurate on a coarse grid indicating that cavity reflections exacerbate false scattering and ray concentration errors and result in an overestimated solar flux on the back tube wall.

Figures 4.3(c) and 4.3(d) reveal only a single peak present in the flux profiles at the cavity wall for an absorbing cavity configuration corresponding to the areas of the cavity wall not shielded from the collimated solar beam. The FV solutions produce a similar peak but it is both broadened and shifted from the location indicated by the MC model. Figures 4.3(a) and 4.3(b) indicate that profiles for the reflective case include both the peak from the first pass solar incidence and others due to specular cavity reflections. The primary FV solution peak becomes

sharper and more distinct as the control angles decrease in size, but retains a significant discrepancy from the MC solution. Only slight improvements are observed as mesh elements are added implying dominance of ray effect errors. All of the FV solutions underestimate the total amount of solar energy incident on the cavity wall because an unrealistically large quantity of the energy is absorbed by the tube after at least one reflection.



Figure 4.3: Profiles of normalized collimated solar energy flux incident on the cavity wall surface for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (c)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity; (d)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

The five tube configuration corresponds to a more realistic receiver design and profiles of normalized solar radiation incident on the cavity wall, center tube, front east tube, and back east tube are shown in Figures 4.4, 4.5, 4.6, and 4.7. The entire cavity wall is shaded from incident collimated radiation by the tube surfaces and, given the high absorptivity of the tube walls, the solutions are nearly identical for both an absorbing and a reflective cavity wall. Only the reflective case is presented here.



Figure 4.4: Profiles of normalized collimated solar energy flux incident on the cavity wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity

The MC solution is nearly zero along the entire length of the cavity wall with slight nonzero values arising from the small diffuse reflectivity of the tube surfaces. FV solutions, on the other hand, exhibit a number of physically unrealistic peaks. Primary peaks at roughly  $\beta = 150^{\circ}$  and  $\beta = 170-180^{\circ}$  result from energy numerically transported between the tubes, and provide a clear representation of the errors inherent in the formulation of the FV method. Secondary peaks at  $\beta = 20^{\circ}$  and  $\beta = 95^{\circ}$  are due to reflection of the primary peaks and are not present in the results for an absorbing cavity. The peaks become sharper as the number of mesh elements increases and false scattering errors are reduced. These non-physical peaks in the cavity wall profiles augment the solar energy incident on the back of the center tube shown in Figure 4.5.


Figure 4.5: Profiles of normalized collimated solar energy flux incident on the center tube wall for: (a)  $(N_{\theta} x N_{\Phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\Phi}) = (15 x 15)$  reflective cavity

Profiles for the outer tubes on the right or east side of the receiver are presented in Figures 4.6 and 4.7. The front tube lies entirely outside of the collimated beam and, as such, the only physically realistic solar incidence originates from diffuse reflections by the other tubes. However, the FV solutions indicate the presence of a large peak in incident energy on the front of the tube arising from a numerical spreading of the initial beam. The back tubes receive a portion of the collimated radiation, but while the MC results show a sharp cutoff at the edge of the aperture the FV solutions fail to capture this discontinuity. Though both false scattering and ray concentration errors are present, it appears that ray concentration errors dominate when  $(N_0 \times N_{\phi}) = (5x5)$  and the solution improves as the number of mesh elements increases, but ray effect errors limit the approach of the approximate FV solution to the nearly exact MC solution. The FV solutions are clearly most accurate for the center tube as the distance between the tube and the window surface is minimized and the majority of the incident solar energy reaches the tube prior to reflection by the cavity wall.



Figure 4.6: Profiles of normalized collimated solar energy flux incident on the front east tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity



Figure 4.7: Profiles of normalized collimated solar energy flux incident on the back east tube wall for: (a)  $(N_{\theta} x N_{\Phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\Phi}) = (15 x 15)$  reflective cavity

#### 4.4.2 Diffuse incident solar radiation

Figure 4.8 illustrates profiles of normalized solar energy flux incident on the tube surface for the single tube geometry with both an absorbing and reflective cavity wall and a uniform diffuse solar input. Only the profiles based on  $(N_{\theta} \times N_{\Phi}) = (15 \times 15)$  are shown here as those based on  $(N_{\theta} \times N_{\Phi}) = (5 \times 5)$  are analogous with only slightly increased solar energy flux on the back side of the tube. The FV solutions for the absorbing cavity agree well with MC solutions whereas the FV solutions for the reflective cavity overestimate the energy incident on the entirety of the tube surface. Thus similar to the case with collimated incident solar energy, the FV method produces a reasonably quantitatively accurate depiction of the energy incident on the tube prior to reflection, but fails to adequately capture the behavior after at least one reflection by the cavity surface.



Figure 4.8: Profiles of normalized diffuse solar energy flux incident on the single tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

Figures 4.9, 4.10, 4.11, and 4.12 display profiles of the normalized radiative flux incident on surfaces in the five tube geometry based on diffuse solar energy originating from the aperture. Peaks in the cavity wall profiles identified via the MC method in Figure 4.9 arise from spacing between the five tubes and the solutions for an absorbing cavity identify regions of the wall which are entirely shielded from incident solar energy. FV results oscillate strongly for  $(N_{\theta} x N_{\phi}) = (5x5)$  and the amplitude of the oscillations increases as the number of mesh elements increases and false scattering no longer compensates for ray effects. Oscillations cannot be attributed to the second-order discretization scheme as identical solutions are obtained with a simple first-order upwind scheme. For the absorbing cavity, the oscillations are roughly centered about the true solution whereas for the reflecting cavity overall solar incidence is marginally underestimated. Solution oscillations disappear for  $(N_{\theta} x N_{\phi}) = (15x15)$  and approach the MC solution as the spatial discretization is refined implying that false scattering errors dominate for  $(N_{\theta} x N_{\phi}) = (15x15)$ .



Figure 4.9: Profiles of normalized diffuse solar energy flux incident on the cavity wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (c)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity; (d)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

For the reflective case, MC solution profiles for the center tube show a slight increase in the solar energy incident on the front of the tube due to reflection from the cavity wall near the aperture. This reflection originates from the small peak in the cavity wall profile at  $\beta \approx 20^{\circ}$  and as the FV solutions do not capture the sharpness of this peak it follows that the FV solutions also

fail to capture the augmented solar energy on the front of the tube. FV solutions are improved with an absorbing cavity and, in this case, highly accurate solutions are possible with sufficient refinement of both spatial and angular grids. Despite the strong oscillations present in the cavity wall profiles for  $(N_{\theta} x N_{\phi}) = (5x5)$ , tube profiles only exhibit slightly larger deviations from the MC profiles compared to those with  $(N_{\theta} x N_{\phi}) = (15x15)$  shown in Figures 4.10, 4.11, and 4.12. Solution profiles at the tube surfaces with  $(N_{\theta} x N_{\phi}) = (25x25)$  are indistinguishable from those in Figures 4.10, 4.11, and 4.12.



Figure 4.10: Profiles of normalized diffuse solar energy flux incident on the center tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

FV solutions for the front tube in Figure 4.11(a) capture peak shape, placement and size, but indicate slightly augmented energy on the back outer side of the tube which cannot be eliminated by improving spatial discretization. The FV solutions in Figure 4.11(b) are highly accurate even on coarse angular and spatial grids and solutions for  $(N_{\theta} x N_{\phi}) = (5x5)$  are indistinguishable from those given in Figure 4.11(b). The FV solutions for the back tube illustrated in Figures 4.12(a) and 4.12(b) fail to capture both the sharpness of a secondary peak at  $\beta \approx -120^{\circ}$  originating from cavity wall reflections, and a region of near zero solar incidence at  $\beta \approx 80-160^{\circ}$  even with a highly refined angular grid. In the case of an absorbing cavity, the basic qualitative profile shape is produced by FV solutions even for  $(N_{\theta} \times N_{\phi}) = (5x5)$  and 2364 mesh elements; however,  $(N_{\theta} \times N_{\phi}) = (15x15)$  and at least 23186 mesh elements are necessary to achieve quantitative accuracy.



Figure 4.11: Profiles of normalized diffuse solar energy flux incident on the front east tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity



Figure 4.12: Profiles of normalized diffuse solar energy flux incident on the back east tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

Reflective cavity solutions for each surface are only marginally improved by increasing the number of spatial mesh elements when  $(N_{\theta} \times N_{\phi}) = (5x5)$  indicating the dominance of ray concentration errors on the coarse angular grid and suggesting that no amount of spatial grid refinement can overcome the deficiencies of the angular grid. For  $(N_{\theta} x N_{\phi}) = (15x15)$  errors due to both false scattering and ray effects are apparent as FV solutions tend toward, but never exactly reach, MC solutions as the number of mesh elements increases. Solutions with  $(N_{\theta} x N_{\phi}) = (25x25)$  and 132453 mesh elements are nearly identical to those with  $(N_{\theta} x N_{\phi}) =$ (15x15) and 83700 elements. For the absorbing case with  $(N_{\theta} x N_{\phi}) = (15x15)$  FV solutions become more accurate as the number of mesh elements increases and closely approach the MC solutions implying that false scattering errors dominate on the coarse spatial mesh. An analogous set of simulations is carried out for incident solar radiation contained within a 30° cone centered about the angle perpendicular to the window. Results are similar to those presented here for collimated radiation, and the overall agreement between the MC and FV solutions lies between the collimated and diffuse cases shown here.

Figures 4.2 – 4.12 suggest that highly reflective enclosure walls exacerbate the errors resulting from the FV formulation. The single tube configuration maximizes cavity wall reflections and, correspondingly, FV solutions are typically less accurate than those for the five tube configuration. FV solutions improve as the character of the incident solar energy changes from collimated to diffuse and FV results with diffuse solar radiation typically approach the MC values but may require both highly refined spatial and angular grids to achieve quantitatively accurate, non-oscillatory solutions. In contrast, FV solutions with collimated solar radiation may never approach MC solution values even on highly refined angular and spatial grids. Solutions with ( $N_{\theta} \times N_{\phi}$ ) = (25 x 25) and 133000 or 132453 mesh elements fail to show significant improvement over the results shown here. Thus use of the FV method to solve the radiative

transfer equation for solar energy in the receiver cavity may prove problematic, particularly for receiver configurations with highly specularly reflective cavity walls or limited absorber area.

### 4.4.3 Solar Absorption Efficiency

The solar absorption efficiencies and corresponding FV method errors for each scenario are shown in Tables 4.4 and 4.5 for, respectively, the single tube and five tube configurations. The absorption efficiency is defined as the fraction of the total solar radiation absorbed by the surface of interest and is calculated from the integral of the normalized flux profile at that surface. For the single tube configuration, the absorption efficiency clearly becomes more accurate as the character of the incident solar radiation tends toward diffuse but errors remain large when the cavity is reflective. Using the spatial and angular grid definitions considered here it is impossible to achieve an absorption efficiency accurate to within 2% of the total solar energy when the cavity is highly reflective. Conversely, with an absorbing cavity this accuracy can, in most cases, be attained on even the coarsest angular and spatial grids. However, accuracy of the absorption efficiency is not necessarily an adequate indication of conformity between FV and MC flux profiles, particularly in the case of oscillatory FV solutions. The cavity wall flux profiles with diffuse solar incidence contain large oscillations when  $(N_{\theta} x N_{\phi}) = (5x5)$  similar to those in Figure 4.9 for the five tube configuration, yet the impact on the absorption efficiency is minimal. The FV solutions for the total energy absorbed by a given surface appear to be more accurate than the distribution of that energy along the surface.

As a whole, the FV absorption efficiencies for the five-tube configuration in Table 4.5 also improve as the character of the solar radiation tends from collimated to diffuse. The FV solutions are typically more accurate than those for the single tube configuration as the presence of additional radiant absorbers effectively limits cavity reflections. With the exception of

collimated solar incidence, it is possible to achieve absorption efficiencies accurate to within 2% of the incident solar energy, though this may require the use of highly refined angular and spatial grids.

				Tube		Cavity Wall				
Beam	Cavity	Elements		$N_{\theta} = N_{\Phi}$		$N_{\theta} = N_{\Phi}$				
			5	15	25	5	15	25		
				$\eta_{abs} = 0.433$	3	$\eta_{abs} = 0.354$				
		2364	0.20	0.24	0.24	-0.15	-0.16	-0.15		
	Refl.	23186	0.21	0.22	0.22	-0.16	-0.14	-0.14		
		83700	0.21	0.20	0.19	-0.16	-0.12	-0.12		
Collimated		133002	0.21	0.20	0.19	-0.16	-0.13	-0.12		
Commateu				$\eta_{abs} = 0.433$	5	1	$\eta_{abs} = 0.556$	ő		
		2364	-0.046	-0.0030	-0.0010	0.012	-0.008	-0.005		
	Abs.	23186	-0.027	0.0004	0.0001	-0.011	-0.011	-0.006		
		83700	-0.024	0.0005	0.0002	-0.014	-0.011	-0.006		
		133002	-0.022	0.0005	0.0002	-0.016	-0.011	-0.006		
				$\eta_{abs} = 0.412$	2	$\eta_{abs} = 0.326$				
		2364	0.22	0.20	0.21	-0.13	-0.11	-0.11		
	Refl.	23186	0.23	0.18	0.18	-0.13	-0.09	-0.09		
		83700	0.23	0.15	0.15	-0.13	-0.07	-0.07		
$30^{\circ}$ cone		133002	0.24	0.15	0.15	-0.13	-0.07	-0.07		
Jo cone				$\eta_{abs} = 0.402$	2	$\eta_{abs} = 0.557$				
		2364	-0.013	-0.021	-0.015	0.010	0.023	0.017		
	Abs.	23186	0.006	-0.012	-0.004	-0.012	0.013	0.006		
		83700	0.009	-0.011	-0.003	-0.015	0.011	0.004		
		133002	0.011	-0.010	-0.002	-0.017	0.010	0.004		
				$\eta_{abs} = 0.13$	$\eta_{abs} = 0.423$					
		2364	0.19	0.16	0.16	-0.084	-0.068	-0.068		
	Refl.	23186	0.16	0.10	0.09	-0.064	-0.036	-0.035		
		83700	0.15	0.08	0.07	-0.062	-0.027	-0.023		
Diffuse		133002	0.15	0.08	0.07	-0.062	-0.025	-0.020		
		22(4	0.000	$\eta_{abs} = 0.129$	)	0.005	$\eta_{abs} = 0.684$	0.002		
	Aba	2364	0.009	0.006	0.006	-0.005	0.003	0.003		
	AUS.	23180 83700	0.007	0.002	0.002	-0.004	0.007	0.007		
		133002	0.007	0.001	0.001	-0.004	0.007	0.007		

Table 4.4: Solar absorption efficiency errors ( $\eta_{abs,FV} - \eta_{abs,MC}$ ) for the single tube configuration

	Beam						=	COII.									200 0000	200 001									D:ff	DIIIUSe				
	Cavity				Refl.					Abs.					Refl.			Abs.				Refl. Abs.										
;	Mesh elements	cicilicitis		3130	23550	80789	132453		3130	23550	80789	132453		3130	23550	80789	132453		3130	23550	80789	132453		3130	23550	80789	132453		3130	23550	80789	132453
		5		-0.002	0.006	0.007	0.009		-0.030	-0.014	-0.011	-0.008		-0.006	0.002	0.003	0.005		-0.012	-0.004	0.008	0.011		0.014	0.005	0.003	0.003		0.009	0.003	0.002	0.002
Center Tube	$N_\theta = N_\Phi$	15	$\eta_{abs} = 0.437$	0.035	0.034	0.028	0.026	$\eta_{abs} = 0.434$	-0.003	-0.0003	-0.0001	-0.0001	$\eta_{abs} = 0.44$	-0.009	-0.005	-0.007	-0.006	$\eta_{abs} = 0.415$	-0.021	-0.012	-0.010	-0.009	$\eta_{abs} = 0.155$	0.012	0.004	0.002	0.002	$\eta_{abs} = 0.139$	0.007	0.002	0.001	0.001
		25		0.037	0.034	0.027	0.024		-0.002	-0.0004	-0.0002	-0.0002		-0.004	0.001	0.0002	0.001		-0.015	-0.005	-0.004	-0.002		0.012	0.004	0.002	0.002		0.007	0.002	0.001	0.001
ł		5		0.075	0.067	0.066	0.065		0.066	090.0	0.059	0.059		0.028	0.020	0.019	0.018		0.019	0.013	0.012	0.012		0.039	0.036	0.035	0.034		-0.0003	0.002	0.002	0.003
Front East Tub	$N_\theta = N_\Phi$	15	$\eta_{abs} = 0.0065$	0.036	0.017	0.013	0.011	$\eta_{abs} = 0.0042$	0.032	0.016	0.012	0.011	$\eta_{abs} = 0.054$	0.024	0.010	0.009	0.006	$\eta_{abs} = 0.051$	0.015	0.007	0.005	0.005	$\eta_{abs} = 0.128$	0.039	0.027	0.021	0.018	$\eta_{abs} = 0.115$	-0.0003	0.002	0.002	0.002
0		25		0.033	0.013	0.008	0.007		0.029	0.012	0.008	0.006		0.021	0.007	0.004	0.003		0.013	0.005	0.003	0.002		0.038	0.026	0.019	0.016		-0.0003	0.002	0.002	0.002
Ц		5		-0.096	-0.089	-0.089	-0.090		-0.12	-0.11	-0.11	-0.11		-0.030	-0.023	-0.023	-0.024		-0.040	-0.030	-0.027	-0.027		0.005	-0.001	-0.002	-0.003		-0.011	-0.008	-0.008	-0.008
3ack East Tu	$N_{\theta} = N_{\Phi}$	15	$\eta_{abs} = 0.270$	-0.066	-0.044	-0.036	-0.032	$\eta_{abs} = 0.268$	-0.079	-0.053	-0.042	-0.038	$\eta_{abs} = 0.204$	-0.022	-0.006	-0.001	-0.0004	$\eta_{abs} = 0.190$	-0.029	-0.014	-0.008	-0.006	$\eta_{abs} = 0.103$	0.002	-0.001	-0.001	-0.0004	$\eta_{abs} = 0.070$	-0.007	-0.003	-0.002	-0.001
be	e 25	25		-0.062	-0.038	-0.029	-0.025		-0.073	-0.044	-0.032	-0.028		-0.022	-0.006	-0.002	-0.001		-0.029	-0.013	-0.008	-0.006		0.002	-0.001	-0.003	-0.0003		-0.007	-0.003	-0.002	-0.001
		5		0.016	0.011	0.010	0.009		660'0	0.074	0.067	0.064		0.008	0.003	0.002	0.002		0.048	0.023	0.016	0.012		-0.032	-0.016	-0.015	-0.013		0.018	0.013	0.011	0.010
Cavity Wall	$N_\theta = N_\Phi$	15	$\eta_{abs} = 0.002$	0.012	0.009	0.007	0.006	$\eta_{abs} = 0.014$	0.087	0.062	0.048	0.042	$\eta_{abs} = 0.009^{2}$	0.008	0.003	0.001	0.001	$\eta_{abs} = 0.065$	0.049	0.024	0.015	0.011	$\eta_{abs} = 0.167$	-0.027	-0.007	-0.004	-0.002	$\eta_{abs} = 0.306$	0.018	0.009	0.007	0.005
		25		0.012	0.008	0.007	0.006		0.084	0.057	0.042	0.035		0.007	0.002	0.001	0.001		0.047	0.022	0.013	0.009		-0.028	-0.008	-0.003	-0.001		0.018	0.009	0.007	0.005

Table 4.5: Solar absorption efficiency errors ( $\eta_{abs,FV} - \eta_{abs,MC}$ ) for the five tube configuration

Adequate depiction of profiles of absorbed solar radiation and relative absorption efficiencies are critically important to predicting the performance of the solar receiver. The mesh element sizes in this study may be unrealistically small for extension to a full three-dimensional simulation required for this purpose. Three-dimensional CFD simulations for the receiver are typically carried out with mesh element cross-sectional sizes comparable to those in the coarsest 2364 or 3130 element mesh used here. Assuming a vertical mesh spacing of 100 elements, the number of equations associated with the three-dimensional FV model exceeds that for the two-dimensional FV model by a factor of 200 leading to potentially prohibitively large computational requirements. Thus while the FV model may provide computational advantages over the MC model in two dimensions, these advantages are unlikely to be retained in three-dimensional configurations unless angular and spatial grids are coarse.

### 4.4.4 Emitted Energy

Net radiative energy present in the receiver cavity is comprised of both the solar component considered above and the energy emitted by heated surfaces. This study focuses on describing radiative energy in the cavity space and, for simplicity, radiation transport through the participating medium contained within each tube is not considered. In order to mimic realistic receiver operation each tube surface is artificially prescribed a non-uniform temperature profile described by equation 4.7 with the highest temperature occurring at the side of the tube facing the aperture.

$$T = T_{\min} + \frac{\Delta T}{2} (\cos \beta + 1)$$
(4.7)

Parameter values are stipulated to be  $\Delta T = 300$  K,  $T_{min} = 1773$  K for the single tube configuration, and  $T_{min} = 1773$  K, 1573 K, and 1373 K for the center, back, and front tubes,

respectively, in the five-tube configuration. Temperature of all cavity wall and aperture surfaces are fixed at 0 K.

Profiles of the radiative energy flux incident on the tube surface in the single tube configuration are shown in Figure 4.13. All profiles of incident radiative energy flux are normalized by the maximum emitted at the highest temperature location. Since the tube lies at the exact center of the cavity, the geometric optical configuration dictates that all emitted energy should be reflected back onto the tube after a single specular reflection unless the emitted energy is lost through the aperture. Figure 4.13 indicates unrealistically low FV solution profiles with a reflective cavity implying that some of the emitted radiation is not reflected back to the tube. Absorption efficiencies defined as a fraction of the total emitted energy are provided in Table 4.6 and, as suggested by the flux profiles, exhibit large errors when the cavity is reflective. Absorption efficiencies for an absorbing cavity are accurate to within 1% of the total emitted radiation even on a coarse mesh.



Figure 4.13: Profiles of normalized emitted energy flux incident on the single tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

The FV solutions are considerably more accurate for the five tube configuration than for the single tube configuration. FV solutions for the cavity wall shown in Figure 4.14 exhibit oscillations on coarse angular and fine spatial grids, thereby illustrating the compensatory effects of ray concentration and false scattering errors. These oscillations are centered at or near MC solutions for both the reflective and absorbing cavity scenarios and only weakly impact the absorption efficiencies listed in Table 4.7. The absorption efficiencies are accurate within 1% of the total emitted radiation on all angular and spatial grids.



Figure 4.14: Profiles of normalized emitted energy flux incident on the cavity wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  reflective cavity; (c)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity; (d)  $(N_{\theta} x N_{\phi}) = (15 x 15)$  absorbing cavity

Despite the oscillations in the cavity wall profiles, tube profiles in Figures 4.15 – 4.17 show only a weak dependence on both the angular and spatial grid and only the solutions with  $(N_{\theta} x N_{\phi}) = (5x5)$  are shown here for brevity.



Figure 4.15: Profiles of normalized emitted energy flux incident on the center tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity



Figure 4.16: Profiles of normalized emitted energy flux incident on the front east tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity



Figure 4.17: Profiles of normalized emitted energy flux incident on the back east tube wall for: (a)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  reflective cavity; (b)  $(N_{\theta} x N_{\phi}) = (5 x 5)$  absorbing cavity

The FV solutions slightly overestimate the energy incident on the front of the center tube and, for the front and back tubes, exhibit profile shapes minimally different than those produced by the MC method. FV solutions generated with an absorbing cavity wall and any angular or spatial grid are nearly indistinguishable from corresponding MC profiles. Absorption efficiencies are accurate to within less than 1% and 0.3% of the total emitted energy for reflective and absorbing cavity configurations, respectively, even on the coarsest angular and spatial grids.

		Center	r Tube	Front Tube				
Cavity	Elements	N <sub>0</sub> =	$= N_{\Phi}$	$N_{\theta} = N_{\Phi}$				
		5	15	5	15			
		$\eta_{abs} =$	0.779	$\eta_{abs} = 0.09$				
Refl.	2364	-0.25	-0.21	0.111	0.091			
	23186	-0.20	-0.13	0.090	0.055			
	83700	-0.19	-0.10	0.085	0.043			
		$\eta_{abs} =$	0.013	$\eta_{abs} = 0.852$				
Abs.	2364	0.0004	0.0004	-0.009	-0.008			
	23186	0.0005	0.0006	-0.001	-0.001			
	83700	0.0006	0.0007	0.001	0.0001			

Table 4.6: Emitted energy absorption efficiency errors  $(\eta_{abs,FV} - \eta_{abs,MC})$  for the single tube configuration

		Cente	r Tube	Front	Tube	Back	Tube	Cavity Wall $N_{\theta} = N_{\Phi}$			
Cavity	Elements	$N_{\theta}$	$= N_{\Phi}$	N <sub>0</sub> =	= $N_{\Phi}$	N <sub>0</sub> =	= $N_{\Phi}$				
		5	15	5	15	5	15	5	15		
		$\eta_{abs} =$	0.176	$\eta_{abs} =$	0.164	$\eta_{abs} =$	0.149	$\eta_{abs} = 0.077$			
Refl.	3130	-0.007	-0.005	-0.007	-0.004	-0.006	-0.006	0.008	0.007		
	23550	-0.002	-0.0002	-0.004	-0.003	-0.003	-0.002	0.005	0.003		
	80789	0.0001	0.001	-0.003	-0.002	-0.002	-0.002	0.004	0.002		
		$\eta_{abs} =$	0.074	$\eta_{abs} =$	0.068	$\eta_{abs}{=}0.056$		$\eta_{abs} =$	0.567		
Abs.	3130	0.0002	0.0005	-0.0027	-0.0029	0.0005	0.0003	-0.0008	-0.0006		
	23550	0.0005	0.0003	-0.0008	-0.0011	0.0003	0.0002	0.0008	0.0006		
	80789	0.0005	0.0003	-0.0002	-0.0006	0.0002	0.0002	0.0005	0.0006		

Table 4.7: Emitted energy absorption efficiency errors  $(\eta_{abs,FV} - \eta_{abs,MC})$  for the five tube configuration

### 4.4.5 Comparison of 3D FV and MC models for the solar component

All comparisons between FV and MC solutions described above are based on calculations for a horizontal two-dimensional slice of the receiver in order to facilitate evaluation of FV solutions on highly refined spatial and angular grids. These grids may not be feasible in a full three-dimensional simulation owing to excessive computational requirements. In order to assess accuracy on realistic mesh element sizes, a full three-dimensional simulation is carried out for the five tube geometry with all solar energy uniformly contained within a 30° cone centered about the angle perpendicular to the window surface. The height of the receiver cavity and window are 28 cm and 9.8 cm respectively, identical to those for the schematic design in Figure 1.1. FV results are evaluated in half of the receiver geometry exploiting the symmetry of the center line with a spatial mesh of 295864 elements and  $(N_{\theta} x N_{\phi}) = (11 x 11)$ . The spatial mesh spacing roughly corresponds to the cross-sectional element sizes utilized in the two-dimensional simulations with 3130 elements. The uniform flux profile is replaced with a Gaussian profile for

solar flux at the aperture surface given by equation 4.8 and a transparent quartz window is utilized in place of an open aperture.

$$q_{s}''\left(\frac{kW}{m^{2}}\right) = 3565.2 \exp\left\{-0.5\left[\left(\frac{y}{0.0192}\right)^{2} + \left(\frac{z}{0.0266}\right)^{2}\right]\right\}$$
(4.8)

The horizontal and vertical positions at the window surface are represented, respectively, by y and z. Figure 4.18 depicts the solar flux incident on the center, front east, and back east tubes from both FV and MC calculations at three vertical positions with z = 0 defined at the aperture centroid. All profiles are normalized to the peak flux at the aperture.



Figure 4.18: Profiles of the normalized solar energy flux incident on the (a) center tube, (b) front tube, (c) back tube from 3D MC and FV models

As expected from two-dimensional calculations, the FV model overestimates the solar energy incident on the front tube and underestimates the solar energy incident on both the center and back tubes. The absorption efficiencies from the MC model are 41.8%, 5.2%, and 17.3% for the center, front and back tubes respectively. The FV model yields corresponding values of 37.8%, 8.7%, and 15.5% and this behavior is consistent with artificial spreading of the initial solar beam. The normalized solar flux incident on the front of the center tube is lower than that predicted by the two-dimensional solutions owing to both reflection at the quartz window surface and the strongly peaked shape of the Gaussian flux profile. The three-dimensional solutions and, correspondingly, solution accuracy is likely numerically improved by the compensatory effects of ray concentration and false scattering errors.

## 4.5 Overall Modeling Strategy

From the preceding results it is evident that FV solutions for the solar radiation component can contain sizeable errors that may negatively impact the distribution of solar energy absorbed by receiver surfaces, particularly in the case of collimated solar radiation. For certain combinations of solar profile, receiver configuration, and cavity wall boundary condition it may be possible to obtain quantitatively accurate solutions with the FV method, but the requisite highly refined angular and spatial grids would likely result in unrealistic computational requirements. Conversely, the main errors present in FV solutions for emitted radiation in the five tube design arise from oscillations present on highly refined spatial grids. Global errors in the FV solutions are minimal and the absorption efficiencies are accurate to within 1% of the total emitted radiation even on coarse angular and spatial grids. For a given receiver geometry, the solar radiation solution can be entirely decoupled from all other heat, mass, and momentum transfer phenomena occurring in the receiver if the surface absorptivity is assumed independent of temperature. A spectral surface absorptivity is still permissible because the distribution of wavelengths is fixed by the blackbody distribution of the sun rather than the temperature of heated surfaces. Therefore the computationally accurate MC method can be used to map the solar radiation onto the tube and cavity surfaces independently of the temperatures of these surfaces. Emitted radiation, on the other hand, is strongly dependent on surface optical properties, temperatures and, correspondingly, all convection and conduction phenomena occurring in the receiver. Thus there are clear computational benefits to using the FV method for emitted radiation as it is directly compatible with control volume based CFD methods and can be solved simultaneously and on the same spatial mesh as the heat, mass and momentum transport equations. Hypothetical use of the MC method for emitted radiation would require a computationally intensive iterative solution of the MC and CFD models.

These results suggest that the optimal approach for solving the radiative transport equation in the solar receiver may be a hybrid scheme employing the MC method for solar incidence while utilizing the FV method to account for emitted radiation. This is similar to the approach used by Baek [18] and Li [30] with the exception that the FV method is introduced to account for radiation emitted by surface elements rather than a participating medium contained within the enclosure. This modeling strategy may not be feasible for single tube receiver configurations with a highly reflective cavity wall as the FV solutions for emitted radiation may be inadequate with minimal absorber area.

# **4.6 Conclusions**

The accuracy of finite volume (FV) radiation models was evaluated for two closed-cavity solar receiver configurations designed for carrying out high temperature solar-thermal reaction processes. The total radiative energy was separated into two components: (1) solar energy introduced through the receiver aperture and (2) energy emitted by heated surfaces within the enclosure. Quantitatively accurate FV solutions for the solar component were not always achievable and required highly refined angular and spatial grids, potentially resulting in unrealistically large computational requirements for full three-dimensional receiver models. However, FV solutions for the emitted energy were sufficiently accurate even on coarse angular and spatial grids. In general, FV solutions improved as cavity reflections were minimized and as the character of the solar energy shifted from collimated to diffuse. Interactions between ray effects and false scattering errors produced oscillations in some heat flux profiles, the amplitude of which increased as the spatial grid was refined. However, these oscillations resulted in minimal impact on the total amount of energy absorbed by a given surface. Ray effect errors dominated on an angular grid specified by  $N_{\theta} x N_{\Phi} = (5x5)$  whereas both ray effect and false scattering errors were evident on angular grids specified by  $(N_{\theta} x N_{\phi}) = (15x15)$  or (25x25). Any sharp peaks and discontinuities present in Monte Carlo (MC) solutions tended to be both broadened and shifted from their original locations by FV solutions. These results suggest an optimal hybrid approach employing the MC method for the solar energy and the FV method for the emitted energy, thereby retaining both the accuracy of the MC method and the compatibility of the FV method with control-volume based CFD heat transfer models where necessary.

### Nomenclature

 $A_s$  control volume face area (m<sup>2</sup>)

а	absorption coefficient $(m^{-1})$
Ι	radiation intensity (W/m <sup>2</sup> /sr)
$I_b$	blackbody intensity (W/m <sup>2</sup> /sr)
$N_f$	number of control volume faces
Nθ	number of divisions of angle $\theta$ per octant
$N_{\Phi}$	number of divisions of angle $\Phi$ per octant
$\vec{n}_f$	vector normal to control volume face
$q_{abs}$	absorbed surface heat flux (W/m <sup>2</sup> )
r	position vector
$\vec{s}$	direction vector
$\vec{S}^{pl}$	pixel solid angle centroid vector
Т	temperature (K)

- $\beta$  angle around tube surface (deg)
- $\varepsilon$  surface emissivity
- $\eta_{abs}$  absorption efficiency
- $\rho$  surface reflectivity
- $\sigma$  Stefan-Boltzmann constant (W/m<sup>2</sup>/K<sup>4</sup>)
- $\sigma_s$  scattering coefficient (m<sup>-1</sup>)
- $\omega$  solid angle
- $\Phi$  scattering phase function

# Subscripts/ Superscripts

- *b* blackbody
- *f* index of control volume face
- *l* index denoting solid angle
- *n* normalized
- *p* index denoting pixel
- w wall

# References

- 1. Siegel, N.P., Ho, C.K., Khalsa, S.S., and Kolb, G.J., Development and Evaluation of a Prototype Solid Particle Receiver: On-Sun Testing and Model Validation. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(2).
- 2. Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., Hydrogen production from solar thermal dissociation of natural gas: development of a 10 kW solar chemical reactor prototype. *Solar Energy*, 2009. **83**(9): p. 1599-1610.
- Haussener, S., Hirsch, D., Perkins, C., Weimer, A., Lewandowski, A., and Steinfeld, A., Modeling of a Multitube High-Temperature Solar Thermochemical Reactor for Hydrogen Production. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2009. 131(2).
- 4. Z'Graggen, A. and Steinfeld, A., A two-phase reactor model for the steam-gasification of carbonaceous materials under concentrated thermal radiation. *Chemical Engineering and Processing*, 2008. **47**(4): p. 655-662.
- 5. Palumbo, R., Keunecke, M., Moller, S., and Steinfeld, A., Reflections on the design of solar thermal chemical reactors: thoughts in transformation. *Energy*, 2004. **29**(5-6): p. 727-744.
- 6. Wieckert, C., Palumbo, R., and Frommherz, U., A two-cavity reactor for solar chemical processes: heat transfer model and application to carbothermic reduction of ZnO. *Energy*, 2004. **29**(5-6): p. 771-787.
- Z'Graggen, A., Haueter, P., Trommer, D., Romero, M., de Jesus, J.C., and Steinfeld, A., Hydrogen production by steam-gasification of petroleum coke using concentrated solar power - II - Reactor design, testing, and modeling. *International Journal of Hydrogen Energy*, 2006. **31**(6): p. 797-811.
- 8. Melchior, T., Perkins, C., Weimer, A.W., and Steinfeld, A., A cavity-receiver containing a tubular absorber for high-temperature thermochemical processing using concentrated solar energy. *International Journal of Thermal Sciences*, 2008. **47**(11): p. 1496-1503.
- 9. Hirsch, D. and Steinfeld, A., Radiative transfer in a solar chemical reactor for the coproduction of hydrogen and carbon by thermal decomposition of methane. *Chemical Engineering Science*, 2004. **59**(24): p. 5771-5778.
- 10. Maag, G., Lipinski, W., and Steinfeld, A., Particle-gas reacting flow under concentrated solar irradiation. *International Journal of Heat and Mass Transfer*, 2009. **52**(21-22): p. 4997-5004.
- 11. Z'Graggen, A. and Steinfeld, A., Hydrogen production by steam-gasification of carbonaceous materials using concentrated solar energy V. Reactor modeling, optimization, and scale-up. *International Journal of Hydrogen Energy*, 2008. **33**(20): p. 5484-5492.

- 12. Raithby, G.D. and Chui, E.H., A Finite-Volume Method for Predicting a Radiant-Heat Transfer in Enclosures with Participating Media. *Journal of Heat Transfer-Transactions of the Asme*, 1990. **112**(2): p. 415-423.
- 13. Chui, E.H. and Raithby, G.D., Computation of Radiant-Heat Transfer on a Nonorthogonal Mesh Using the Finite-Volume Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **23**(3): p. 269-288.
- 14. Truelove, J.S., 3-Dimensional Radiation in Absorbing Emitting Scattering Media Using the Discrete-Ordinates Approximation. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1988. **39**(1): p. 27-31.
- 15. Fiveland, W.A., Discrete Ordinate Methods for Radiative Heat-Transfer in Isotropically and Anisotropically Scattering Media. *Journal of Heat Transfer-Transactions of the Asme*, 1987. **109**(3): p. 809-812.
- 16. Chai, J.C., Lee, H.S., and Patankar, S.V., Ray Effect and False Scattering in the Discrete Ordinates Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **24**(4): p. 373-389.
- 17. Raithby, G.D., Evaluation of discretization errors in finite-volume radiant heat transfer predictions. *Numerical Heat Transfer Part B-Fundamentals*, 1999. **36**(3): p. 241-264.
- 18. Baek, S.W., Byun, D.Y., and Kang, S.J., The combined Monte-Carlo and finite-volume method for radiation in a two-dimensional irregular geometry. *International Journal of Heat and Mass Transfer*, 2000. **43**(13): p. 2337-2344.
- 19. Byun, D.Y., Baek, S.W., and Kim, M.Y., Thermal radiation in a discretely heated irregular geometry using the Monte-Carlo, finite volume, and modified discrete ordinates interpolation method. *Numerical Heat Transfer Part a-Applications*, 2000. **37**(1): p. 1-18.
- 20. Chai, J.C., Hsu, P.F., and Lam, Y.C., Three-dimensional transient radiative transfer modeling using the finite-volume method. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2004. **86**(3): p. 299-313.
- 21. Coelho, P.J., The role of ray effects and false scattering on the accuracy of the standard and modified discrete ordinates methods. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2002. **73**(2-5): p. 231-238.
- 22. Koo, H.M., Vaillon, R., Goutiere, V., Le Dez, V., Cha, H., and Song, T.H., Comparison of three discrete ordinates methods applied to two-dimensional curved geometries. *International Journal of Thermal Sciences*, 2003. **42**(4): p. 343-359.
- 23. Sakami, M. and Charette, A., Application of a modified discrete ordinates method to twodimensional enclosures of irregular geometry. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2000. **64**(3): p. 275-298.

- 24. Tan, H.P., Zhang, H.C., and Zhen, B., Estimation of ray effect and false scattering in approximate solution method for thermal radiative transfer equation. *Numerical Heat Transfer Part a-Applications*, 2004. **46**(8): p. 807-829.
- 25. Li, H.S., Flamant, G., and Lu, J.D., Mitigation of ray effects in the discrete ordinates method. *Numerical Heat Transfer Part B-Fundamentals*, 2003. **43**(5): p. 445-466.
- 26. Howell, J.R., The Monte Carlo method in radiative heat transfer. *Journal of Heat Transfer-Transactions of the Asme*, 1998. **120**(3): p. 547-560.
- 27. Siegel, R. and Howell, J., *Thermal Radiation Heat Transfer*. 4 ed. 2002, New York: Taylor and Francis.
- 28. Lichty, P., Perkins, C., Woodruff, B., Bingham, C., and Weimer, A., Rapid High Temperature Solar Thermal Biomass Gasification in a Prototype Cavity Reactor. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(1): p. -.
- 29. Murthy, J.Y. and Mathur, S.R., Finite volume method for radiative heat transfer using unstructured meshes. *Journal of Thermophysics and Heat Transfer*, 1998. **12**(3): p. 313-321.
- 30. Li, H.S. and Werther, J., Computation of radiative image formation in isolated source and collimated irradiation problems. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2006. **97**(1): p. 142-159.

# **Chapter V**

Computational modeling and on-sun model validation for a multiple tube solar aerosol flow reactor with specularly reflective cavity walls

### 5.1 Abstract

A three-dimensional, steady state computational model coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics is developed for a solar receiver consisting of a specularly reflective cylindrical cavity with a windowed aperture enclosing an array of five tubes. Radiation heat transfer is incorporated via a combination of ray tracing, Monte Carlo, and finite volume methods. Ray trace modeling of the concentrating system provides the magnitude and direction of solar energy incident on the window surface. Transport of solar radiation in the cavity space is decoupled from all other transport processes occurring in the receiver and profiles of the absorbed solar energy are determined via a Monte Carlo technique requiring only the receiver geometry, magnitude and direction of radiative energy incident on the window, and spectral directional optical properties. A finite volume model is implemented in conjunction with a computational fluid dynamics model to account for thermal radiation emitted by heated surfaces in the receiver. Steam gasification of 42 nm acetylene black particles is considered with particle transport dictated by an aerosol population balance featuring convection, Brownian motion, and thermophoretic diffusion. Maximum temperatures of 1813 K, 1343 K and 1546 K are predicted for the center, front and back tubes respectively, with corresponding reaction conversion of 40%, 2.5% and 9.2% for a solar power input of 6 kW. Temperature gradients as high as 340 K develop between the front and back sides of the center tube, while fluid and particle temperatures track closely with wall temperatures due to radiative absorption by the particulate phase. Estimated receiver efficiency ranges between 1-4% depending on operating conditions though more than 79% of the solar energy is absorbed by tube surfaces. Emission losses, including absorption of emitted energy by cooled surfaces, account for 11-25% of the solar energy whereas conductive heat losses account of 55-69% of the solar input and primarily result from conduction along the tube length into receiver cooling zones. Results from the computational model are validated with on-sun experimental temperature and reaction conversion measurements. Average discrepancies between predicted and measured temperatures are 44 K (4%) for silicon carbide and 21 K (2%) for Inconel tubes over temperature ranges of 600-1700 K and 700-1400 K respectively.

### **5.2 Introduction**

Concentrated solar energy can be used to provide the heat necessary to drive various highly endothermic chemical reactions for renewable fuel production including direct thermolysis of water, thermal reduction of metal oxides for production of hydrogen via water splitting cycles, carbothermal reduction of metal oxides, thermal dissociation of methane, and gasification of cellulosic biomass, coal or other carbonaceous materials to produce synthesis gas [1-3]. Metal oxide cycles and biomass gasification, when powered by the clean energy of the sun, are theoretically entirely renewable and carbon neutral. Yet the inherent advantages of these processes cannot be exploited on a large scale without detailed knowledge and fundamental understanding of the solar receiver. Numerous solar reactor concepts have been proposed [4-11] with most consisting of cavity-receiver type designs in which concentrated solar radiation enters into a closed cavity through a small aperture or window. Computational models of these receivers can be used to characterize receiver performance and accurate descriptions of receiver

transport phenomena involve coupling typical momentum, continuity, and energy equations with the complex integro-differential equations describing radiative transfer. Finite volume or discrete ordinates, [4, 8, 12, 13] radiosity, [7, 10] and Monte Carlo [6, 11, 14, 15] methods are commonly employed to solve the radiative transfer problem. In receiver modeling studies, use of the MC technique typically comes at the expense of complexity in fluid flow and heat transfer models which are commonly simplified to one-dimensional equations or global/macroscopic models [6, 14, 15] with constant properties. In contrast, the finite volume (FV) [16, 17] and discrete ordinates (DO) [18] methods retain compatibility with a control-volume based CFD modeling approach and thus FV/DO radiation models are commonly implemented in conjunction with highly complex three-dimensional fluid flow and heat transfer models including, for instance, discrete particle models, turbulence, and the effects of buoyancy [4, 8]. However, calculations detailed in Chapter 4 clearly indicate inadequacies in solutions obtained via the finite volume method for solar energy in the receiver cavity due to ray concentration and false scattering errors. Similar deficiencies have been detailed in the literature for cases with isolated heat sources, non-participating media, highly reflective boundary surfaces, and collimated radiative energy [19-22].

The solar receiver described by Lichty et al. [5] consists of a reflective cylindrical outer cavity constructed of polished aluminum with an inner diameter of 18.3 cm. A rectangular quartz window (5.7 cm by 9.8 cm) sits at the front of the cavity and is surrounded by a nickel-plated copper cooling plate. The receiver may be operated either open to the atmosphere with a windowless aperture, or sealed from the surrounding environment by means of a quartz window in order to prevent oxidation of the tube material. The cavity encloses five interchangeable 2.54 cm outer-diameter, 0.356 m long flow tubes arranged in the staggered pattern shown in Figure

1.1. Each tube extends 3.8 cm above and below the vertical extent of the cavity. Cooling zones encircle the top, bottom, front, back, and window and were designed such that cooling fluid flows immediately behind all reflective surfaces to prevent overheating or oxidation of polished aluminum cavity walls. Detailed positioning of the tubular array was specified in Figure 4.1(b).

The focus of the current study is on the development of a highly accurate computational model for the reflective cavity receiver capable of quantitatively predicting receiver temperature profiles, reaction conversion, and solar-to-chemical efficiency. The receiver model must couple heat, mass, momentum and radiation transport models with an accurate depiction of chemical kinetics for the reactant species. Kinetics of biomass pyrolysis and gasification are poorly understood over the elevated temperature range of interest and most models reported in the literature represent simplified global reactivity descriptions which lump intrinsic surface kinetics with heat and mass transfer processes. As such, these simplified global models produce apparent kinetic parameters which have, at best, limited applicability to disparate materials and conditions [23, 24]. Gasification kinetics of pure carbon, low-ash coal chars, and petcoke are comparatively simpler and, consequently, gasification of pure carbon is used in this study as a test reaction in lieu of biomass char.

### **5.3 Radiation Model**

### 5.3.1 Characterization of the solar flux profile

The solar flux incident on the aperture or window surface is produced by the High Flux Solar Furnace (HFSF) at the National Renewable Energy Laboratory (NREL). The HFSF is described by Lewandowski et al. [25] and consists of a single flat heliostat with a 31.8 m<sup>2</sup> surface area, a primary concentrator comprised of an array of 25 mirrored hexagonal facets each

with an identical 14.6 m spherical radius of curvature, and a vertically-opposing two plate attenuator utilized to control the total power incident on the receiver with a maximum achievable solar input of roughly 9 kW. The secondary concentrator described by Dahl et al. [26] is placed in front of the receiver aperture. This concentrator narrows from an octagonal inlet to a rectangular outlet with dimensions matching those of the aperture and is capable of producing more than 3000 kW/m<sup>2</sup> peak flux with a fully open attenuator. A ray-tracing model of the HFSF developed in the program SolTrace [27] provides characterization of the solar flux incident on the window surface. A large number of rays are generated at random based on the position of the sun and tracked through each stage of the concentration system, eventually yielding the position and direction of every ray at the receiver aperture surface. The ray-tracing model includes opaque surfaces defined by the heliostat, primary concentrator, attenuator, and secondary concentrator with uniform reflectivities of, respectively, 0.925, 0.855, 0, and 0.73. Degradation of the reflective secondary concentrator surface from its original condition produces uncertainty in the realistic surface optical properties and the reflectivity is chosen such that the estimated total power at the exit plane from the ray-tracing model matches closely with that measured using a blackbody calorimeter as a function of attenuator opening. The secondary concentrator exit plane is placed at the focal point of the primary concentrator with a transparent plane representing the receiver aperture situated 1.5 cm behind the focal point along the optical axis. This arrangement corresponds with approximate alignment during experimental operation.

The solar flux profile is derived from distributions of locations at which rays intersect the plane representing the aperture or window surface. Flux profiles with 100%, 50%, and 25% attenuator opening are illustrated in Figure 5.1. Each profile is strongly peaked in the center of the aperture and remains higher at the edges of the horizontal (x) dimension than the vertical (y)

dimension. The magnitude of the peak flux scales as a function of attenuator opening decreasing from roughly 3200 kW/m<sup>2</sup> to 1200 kW/m<sup>2</sup> as the attenuator opening narrows from 100% to 25%, whereas the profile shape remains relatively unaffected. Slight asymmetry evident in the profiles originates from the off-axis design of the HFSF and experimentally produces marginally higher temperatures in the east half of the receiver described by a positive *x*-coordinate.



Figure 5.1: Solar flux (kW/m<sup>2</sup>) at the window surface with an attenuator opening of (a) 100%, (b) 50%, (c) 25%

Distributions of the directions at which rays strike the receiver window are a complex function of geometric position and attenuator opening. Each ray can be described by an angle relative to the horizontal *x*-axis ( $\omega$ ) and the vertical *y*-axis ( $\gamma$ ) measured from the negative side of the axis as shown in Figure 5.2. Figure 5.2 denotes the corresponding angle  $\gamma' = 180^\circ - \gamma$ . Note that the coordinate system described here is chosen for convenience with the SolTrace model and does not directly correspond to that employed with the Monte Carlo model described in Chapter 3.



Figure 5.2: Coordinate system for description of ray directions at the aperture

Figure 5.3 depicts heat image maps indicating the relative number of rays incident on the aperture within discrete ( $\omega$ ,  $\gamma$ ) interval combinations for attenuator openings of 100%, 50%, and 25% with a specified uniform interval size of 0.5° for each angle. Figure 5.3 is generated utilizing all rays striking the aperture and darker colors denote a larger number of rays contained within a given  $(\omega, \gamma)$  interval. Hexagonal shapes visible in Figure 5.3 are clear images of the 25 primary concentrator facets and imply that each facet of the primary concentrator generates a specific set of  $(\omega, \gamma)$  combinations. While most ray angles are contained within a primary band centered about the direction perpendicular to the window ( $\omega = \gamma = 90^\circ$ ), secondary bands containing both acute and obtuse angles are produced by reflections from the secondary concentrator and are most prominent in the angle  $\omega$  measured relative to the horizontal. As the attenuator opening decreases, the line of sight between the aperture and upper and lower primary concentrator facets is cut off thereby reducing the solar incidence. The top and bottom facets produce the largest and smallest  $\gamma$  angles in the primary band and thus the distribution of  $\gamma$  angles narrows considerably as the attenuator opening decreases while the distribution of  $\omega$  angles remains relatively unaffected.



Figure 5.3: Angles describing ray directions for energy incident on the entire window surface with an attenuator opening of (a) 100%, (b) 50%, (c) 25%

Angles dictating ray direction are defined such that rays described by  $\omega < 90^{\circ}$  are directed in the positive *x* direction and those described by  $\omega > 90^{\circ}$  are directed in the negative *x* direction as shown in Figure 5.2. Figure 5.4 illustrates variability in ray directions as a function of horizontal position on the window surface for an attenuator opening of 50%. Each image represents ray directions for solar energy incident on a third of the window area from the left (-*x*) to the right side of the window (+*x*). Near the edges of the window the secondary bands at  $\omega = 120-150^{\circ}$  (-*x*) and  $\omega = 30-60^{\circ}$  (+*x*) direct the solar energy toward the edges of the cavity and away from the

tube array. Only minor variability is discernible between images representing solar energy incident on the window at different vertical positions.



Figure 5.4: Angles describing ray direction for solar energy incident on the window between: (a) -2.86 cm < x < -0.95 cm, (b) 0.95 cm < x < 2.86 cm, (c) -0.95 cm < x < 0.95 cm

### 5.3.2 Modeling strategy for radiation in the receiver cavity

Results in Chapter 4 indicate that finite volume solutions for the solar component can contain sizeable errors that may negatively impact the distribution of energy absorbed by receiver surfaces, particularly in the case of collimated solar radiation. Though it may be possible to obtain quantitatively accurate solutions with the finite volume method for certain combinations of solar profile, receiver configuration, and cavity wall boundary condition, the

120

requisite highly refined angular and spatial grids would result in unrealistic computational requirements for 3D simulations. Conversely, inaccuracy in finite volume solutions for emitted radiation in the five tube design arises primarily from oscillations present on refined spatial grids. Global errors in the 2D finite volume solutions detailed in Chapter 4 were minimal and the absorption efficiencies were accurate to within 1% of the total emitted energy even on coarse angular and spatial grids.

For a given receiver geometry, the solar radiation solution can be entirely decoupled from all other heat, mass, momentum and chemical reaction phenomena occurring in the receiver if the surface absorptivity is assumed independent of temperature. A spectral surface absorptivity is still permissible because the distribution of wavelengths is independently fixed by the blackbody distribution of the sun rather than the temperature of receiver surfaces. Therefore the computationally accurate Monte Carlo method can be used to map solar energy onto the tube and cavity surfaces independently of the temperatures of these surfaces. Emitted radiation, on the other hand, is strongly dependent on surface optical properties, temperatures and, correspondingly, all convection and conduction phenomena occurring in the receiver. Thus there are clear computational benefits to using the finite volume method for emitted radiation as it is directly compatible with control volume based computational fluid dynamics (CFD) methods and can be solved simultaneously and on the same mesh as the heat, mass and momentum transport equations. Based on these results, a hybrid approach was selected employing the Monte Carlo method for solar radiative energy while utilizing the finite volume method to account for emitted energy. This approach retains both the computational accuracy of the Monte Carlo model for the solar component and the CFD compatibility of the finite volume method for the emitted component.

#### 5.3.3 Monte Carlo model for solar radiation

The 3D Monte Carlo ray tracing model detailed in Chapter 3 is applied for solar energy entering the cavity though the receiver window. The solar energy impinging on the exterior window surface is discretized into a large number of rays and the stochastic path of each ray is followed as it travels through the receiver cavity and interacts with various boundary surfaces. As the medium within the cavity space is assumed non-participating, only absorption and reflection by boundary surfaces are considered. The initial position and direction of each ray is chosen at random from the shape of the flux profile and probability distributions describing incident angles produced by the SolTrace model. All probability distributions are generated as a function of attenuator opening and thus the magnitude and directionality of the flux profile at the window surface vary with the total solar power incident on the receiver. Specification of initial ray positions proceeds via equations 3.10 and 3.11 with both horizontal and vertical window dimensions divided into 20 intervals. The discrete probability distributions describing ray directions are generated with each vertical and horizontal spatial window dimensions divided into 10 intervals and  $n_{angle} = 90$ . Each window surface element has an independent joint probability function describing incident angles  $\omega$  and  $\gamma$  leading to random specification of each ray direction via equations 3.14-3.20. Spectral, directional reflectivity of the specular cavity wall is estimated from electromagnetic theory using the complex index of refraction of the surface material as detailed in Chapter 3. All tube and cavity surfaces are divided into discrete facets with the energy flux at each element computed from the surface area and the number of rays incident on or absorbed by the element. Cavity and tube walls are discretized into, respectively, 20,000 and 10,000 uniformly sized elements.

The Monte Carlo model is detailed mathematically in Chapter 3 and is implemented in MATLAB<sup>®</sup>. Table 5.1 provides the maximum and average discrepancies between repeated simulations for absorption efficiency and absorbed solar energy flux as a fraction of the peak flux at the aperture and as a function of the number of rays. The absorption efficiency is defined as the fraction of solar energy absorbed by a given tube surface. Based on the results in Table 5.1, all subsequent simulation results are obtained with  $10^7$  rays.

	Error i	Error in absorption				
# rays	(fraction of pea					
	Maximum	efficiency				
$10^{4}$	0.405	0.013	0.011			
10 <sup>5</sup>	0.136	0.004	0.003			
$10^{6}$	0.042	0.002	0.0004			
10 <sup>7</sup>	0.024	0.0008	0.0003			

Table 5.1: Maximum and average errors in absorbed solar flux

Profiles of solar energy flux absorbed around each tube surface in a horizontal plane aligned with the aperture centroid are illustrated in Figure 5.5 for a 50% attenuator opening yielding 6 kW total solar power. The angle  $\beta$  is measured counterclockwise from the direction facing the aperture. All tube profiles are strongly peaked with minimal solar energy received by the back portion of any tube. A minor secondary peak at the back side of the back tubes results from reflected energy and the east (E) and west (W) designation relates to outer tubes described by a positive and negative *x*-coordinate, respectively.

Profiles of solar energy incident on the cavity wall surface are shown in Figure 5.6 at a horizontal plane aligned with aperture centroid. Distinct peaks in the cavity wall profile arise from spacing between the tubes in the array, and the comparatively low flux values indicate that


Figure 5.5: Solar energy flux absorbed by the tubes in a horizontal plane aligned with the aperture centroid



Figure 5.6: Solar energy flux incident on the cavity wall in a horizontal plane aligned with the aperture centroid

Figure 5.7 reveals that a decrease in attenuator opening produces only minimal variability in profiles of absorbed solar energy normalized by the peak flux at the window surface for the

center tube in the horizontal plane aligned with the aperture centroid. Conversely, the normalized solar energy flux absorbed in the plane aligned with the top of the window decreases with attenuator opening as a result of the narrowing range of angle  $\gamma$  illustrated in Figure 5.4. Based on these results, a slight decrease in heated length can be expected at low solar power.



Figure 5.7: Normalized solar energy flux absorbed by the center tube as a function of vertical position and attenuator opening

Fractional absorption efficiencies and reflection losses are displayed in Table 5.2 as a function of attenuator opening. Absorption efficiency is defined as the fraction of the total solar power absorbed by a given surface and is not appreciably altered by attenuator opening. Thus while the local distribution of solar energy absorbed along a given surface may vary with attenuator opening, particularly in planes nearing the vertical extents of the aperture, the global distribution of solar energy between tubes remains essentially unchanged. This comes as a consequence of the relative constancy in the distribution of angle  $\omega$  compared to that of  $\gamma$  with respect to attenuator opening illustrated in Figure 5.3. Reflection losses at the exterior window surface account for 4.7% of the solar energy, whereas losses arising from reflection by the cavity wall or interior window surface increase from 8-9.5% of the total solar energy as the attenuator opening

decreases. Nearly 80% of the solar energy incident on the external window surface is eventually absorbed by one of the receiver tubes and the discernible east/west discrepancy originates from flux profile asymmetry.

Attenuator opening (%)	Power (kW)	Absorption efficiency							<b>Reflection losses</b>	
		Center tube	Front east tube	Front west tube	Back east tube	Back west tube	Cavity wall	Exterior window surface	Cavity wall or interior window surface	
10	1.2	0.327	0.079	0.069	0.164	0.154	0.068	0.046	0.094	
25	3.0	0.326	0.079	0.069	0.166	0.153	0.073	0.047	0.087	
35	4.2	0.328	0.078	0.068	0.164	0.153	0.078	0.047	0.084	
50	5.9	0.328	0.078	0.068	0.165	0.153	0.080	0.048	0.080	

Table 5.2: Solar absorption efficiencies and reflection losses as a function of attenuator opening

Figure 5.8 shows the solar energy flux absorbed by the center tube, front east tube, and back east tube in the horizontal plane aligned with the aperture centroid after at least one reflection by the cavity wall.



Figure 5.8: Solar energy flux absorbed after reflection

Clearly absorption of solar energy by the tube array occurs predominantly prior to interaction of that energy with the cavity wall. Cavity wall reflections serve to weakly augment the solar incidence on the back of the back tubes or the front of the center tube after, respectively, one or two specular reflections. First pass absorption efficiencies are 0.314, 0.072, 0.061, 0.154, and 0.141 for the center, front east, front west, back east and back west tubes, respectively, signifying that 90-95% of solar absorption occurs prior to reflection.

### 5.3.4 Finite volume model for emitted energy

The finite volume radiation model is utilized to account for energy emitted by the heated tube surfaces both into the cavity space and into the tube interior. The finite volume model provides an approximate solution to the radiative transfer equation (RTE) which describes the change in radiation intensity along a path *s* due to absorption, scattering, and emission [28].

$$\frac{dI_{\lambda}(\vec{r},\vec{s})}{dS} = -(a_{\lambda} + \sigma_{s\lambda})I_{\lambda}(\vec{r},\vec{s}) + a_{\lambda}I_{\lambda b}(\vec{r}) + \frac{\sigma_{s\lambda}}{4\pi} \int_{0}^{4\pi} I_{\lambda}(\vec{r},\vec{s}')\Phi(\vec{s},\vec{s}')d\omega'$$
(5.1)

In equation 5.1  $I_{\lambda}$  represents the directional spectral radiative intensity,  $a_{\lambda}$  and  $\sigma_{s\lambda}$  are, respectively, the spectral absorption and scattering coefficients of the medium,  $I_{\lambda b}$  is the directional spectral blackbody intensity, and  $\Phi$  is the scattering phase function. The vectors  $\vec{r}$  and  $\vec{s}$  denote, respectively, the spatial position and path of the radiation whereas *S* represents the coordinate along the path of radiation

The finite volume technique is implemented in the commercial software ANSYS FLUENT version 6.3.26 which exploits the finite volume scheme of Chui and Raithby and its extension to unstructured meshes [16, 17, 29]. The finite volume (FV) method divides each octant of space into  $N_{\theta} \ge N_{\varphi}$  control angles with constant  $\theta$  and  $\varphi$  extents with intensity taken to

be uniform over each solid angle. The RTE is integrated over control volume p and solid angle  $\omega^l$ , yielding, with no solid angle overhang:

$$\sum_{f=1}^{N_f} A_{s,f} I_{if}^{\ell} \vec{n}_f \cdot \int_{\omega^{\ell}} \vec{s} d\omega = \left[ \left( -a_p + \sigma_{s,p} \right) I_p^{\ell} + a_p I_{b,p} + \frac{\sigma_{s,p}}{4\pi} \sum_{\ell'} I_p^{\ell'} \Phi(\ell,\ell') \omega^{\ell'} \right] V_p \omega^{\ell}$$
(5.2)

where  $N_f$  is the number of faces on control volume p,  $A_{s,f}$  is the area of face f,  $I_{if}^{l}$  is the discrete intensity at face f within solid angle  $\omega^{l}$ ,  $\vec{n}_{f}$  is the surface normal vector of control volume face f,  $a_p$  and  $\sigma_{sp}$  are, respectively, the absorption and scattering coefficients of the medium in control volume p,  $I_p^{l}$  is the discrete intensity in control volume p within solid angle  $\omega^{l}$ ,  $I_{b,p}$  is the blackbody intensity in control volume p, and  $V_p$  is the volume of control volume p. The direction  $\vec{s}$  is given in the global Cartesian coordinate system in terms of spherical zenith and azimuth angles  $\theta$  and  $\varphi$  as:

$$\vec{s} = (\sin\theta\cos\phi)\hat{i} + (\sin\theta\sin\phi)\hat{j} + (\cos\theta)\hat{k}$$
(5.3)

The extent of solid angle  $\omega^l$  is calculated from equation 5.4 where  $\theta^l$  is the zenith angle representing the centroid of the solid angle.

$$\omega^{\ell} = \int_{\Delta\phi} \int_{\Delta\theta} \sin\theta d\theta d\phi = 2\sin\theta^{\ell} \sin\left(\frac{\Delta\theta}{2}\right) \Delta\phi$$
(5.4)

When control angle boundaries are not aligned with mesh faces the intensity is subdivided into incoming and outgoing intensities through the use of pixelization for each control angle [29]. Each control angle is divided into  $N_{\theta p} \ge N_{\Phi p}$  auxiliary solid angles and the analogous form of the left hand side of equation 5.2 is provided in equation 5.5 where the integrals are carried out over the extents of the pixel solid angles and are purely geometric factors which can be evaluated analytically in terms of directions in the global coordinate system and solid angle extents.

$$\sum_{f=1}^{N_f} A_{s,f} \left( I_{if,out}^{\ell} \vec{n}_f \cdot \sum_{\vec{s}^{p\ell} \cdot \vec{n}_f > 0} \int_{\omega^{p\ell}} \vec{s} d\omega + I_{if,in}^{\ell} \vec{n}_f \cdot \sum_{\vec{s}^{p\ell} \cdot \vec{n}_f < 0} \int_{\omega^{p\ell}} \vec{s} d\omega \right)$$
(5.5)

The interior summations are carried out over all pixels within a control angle and directions  $\vec{s}^{p\ell}$  represent the direction of the pixel solid angle centroids. Spatial discretization schemes are necessary to relate intensity values at the control volume faces  $(I_{if}^{l})$  to nodal values  $(I_{p}^{l})$ . In this study a second order upwind discretization scheme is employed and the face values are computed from the nodal value and the gradient in the upwind control volume. All gradients are approximated using a Green-Gauss node-based evaluation.

The finite volume model is utilized only for radiative energy emitted by heated surfaces within the receiver. All tube and cavity surfaces are assigned uniform hemispherical optical properties and spectral or directional dependencies are ignored in order to minimize computational intensity. Directional reflectivity at the quartz window interface is calculated from Fresnel's equation (equation 3.25). The outgoing intensity for an opaque diffuse-gray emitting and reflecting boundary is given by equation 5.6 [28].

$$I(r_{w},\vec{s}) = \varepsilon_{w}I_{b} + \frac{1 - \varepsilon_{w}}{\pi} \int_{\vec{s}'\cdot\vec{n}_{w}<0} I(r_{w},\vec{s}') |\vec{s}'\cdot\vec{n}_{w}| d\omega$$
(5.6)

The outgoing intensity for an opaque specularly reflecting boundary is given by equation 5.7 with reflected ( $\vec{s}$ ) and incident ( $\vec{s}$ ') directions related by equation 5.8.

$$I(r_w, \vec{s}) = \varepsilon_w I_b + (1 - \varepsilon_w) I(r_w, \vec{s}')$$
(5.7)

$$\vec{s}' = \vec{s} - 2(\vec{s} \cdot \vec{n}_w)\vec{n}_w \tag{5.8}$$

Figure 5.9 illustrates the relationship between incident, reflected, and transmitted refracted radiative energy for specularly reflecting semi-transparent boundaries such as the quartz window with refractive indices  $n_a < n_b$ .



Figure 5.9: Specification of incident, reflected, and transmitted directions for semi-transparent boundaries

The outgoing intensity at the interface can be described by equations 5.9 and 5.10 in which incident and reflected directions are related by equation 5.8 and incident and transmitted directions are related by Snell's law. Directional reflectivity is approximated from the index of refraction of the material via electromagnetic theory.

$$I_{a}(r_{w},\vec{s}) = \rho_{a}(\vec{s}')I_{a}(r_{w},\vec{s}') + [1 - \rho_{b}(\vec{s}_{t})]I_{b}(r_{w},\vec{s}_{t}) \qquad \theta_{b} < \sin^{-1}\frac{n_{a}}{n_{b}}$$
(5.9)

$$I_{a}(r_{w},\vec{s}) = \rho_{a}(\vec{s}')I_{a}(r_{w},\vec{s}') \qquad \theta_{b} \ge \sin^{-1}\frac{n_{a}}{n_{b}} \qquad (5.10)$$

The gaseous medium filling the cavity space is assumed non-participating while the twophase mixture flowing through each tube can potentially absorb and scatter the incoming radiative energy. Absorption and scattering parameters associated with small particles entrained in the gas phase are calculated from Mie theory. Absorption and scattering coefficients for the suspension are calculated from those for a single particle derived from superposition of analytical solutions to Maxwell's equation in the interior of a spherical particle and within the surrounding medium under assumptions of a homogeneous particle material, a non-absorbing external medium, and elastic scattering [30]. Absorption and scattering efficiencies are defined as the ratio of the absorption or scattering cross section to the geometric projected area of the sphere and are given by equations 5.11-5.14 where  $Q_{sca}$  is the scattering efficiency,  $Q_{abs}$  is the absorption efficiency, *m* is the complex refractive index of the particle divided by that of the surrounding medium, and  $\psi_n$  and  $\xi_n$  are Riccati-Bessel functions [30].

$$Q_{sca} = \frac{2}{\xi^2} \sum_{n=1}^{\infty} (2n+1) \left[ \left| a_n \right|^2 + \left| b_n \right|^2 \right]$$
(5.11)

$$Q_{abs} = \frac{2}{\xi^2} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}\{a_n + b_n\} - \frac{2}{\xi^2} \sum_{n=1}^{\infty} (2n+1) \left[ \left| a_n \right|^2 + \left| b_n \right|^2 \right]$$
(5.12)

$$a_{n} = \frac{m\psi_{n}(mx)\psi_{n}(x) - \psi_{n}(x)\psi_{n}(mx)}{m\psi_{n}(mx)\xi_{n}(x) - \xi_{n}(x)\psi_{n}(mx)}$$
(5.13)

$$b_{n} = \frac{\psi_{n}(mx)\psi_{n}(x) - m\psi_{n}(x)\psi_{n}(mx)}{\psi_{n}(mx)\xi_{n}(x) - m\xi_{n}(x)\psi_{n}(mx)}$$
(5.14)

The particle size parameter  $\xi$  is given by equation 5.15 where  $d_p$  is the diameter of the spherical particle, and  $\lambda_m$  is the wavelength of the incident energy in the surrounding medium.

$$\xi = \frac{\pi d_p}{\lambda_m} \tag{5.15}$$

The scattering phase function can be calculated from Mie theory using equations 5.16-5.18 where  $P_n^{\ l}$  are associated Legendre polynomials with m = 1 [30].

$$\Phi = \frac{|S_1|^2 \sin^2 \theta + |S_2|^2 \cos^2 \theta}{\pi \xi^2 Q_{sca}}$$
(5.16)

$$S_1 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[ a_n \frac{P_n^1(\cos\theta)}{\sin\theta} + b_n \frac{dP_n^1(\cos\theta)}{d\theta} \right]$$
(5.17)

$$S_2 = \sum_{n=1}^{\infty} \frac{2n+1}{n(n+1)} \left[ a_n \frac{dP_n^1(\cos\theta)}{d\theta} + b_n \frac{P_n^1(\cos\theta)}{\sin\theta} \right]$$
(5.18)

Absorption efficiency, scattering efficiency, and scattering phase function for a single particle are calculated in MATLAB via Mie theory using the complex index of refraction of the particle material and the BHMIE algorithm [30]. For ease of computation, the scattering phase function

from Mie theory is fit to a two parameter Delta-Eddington form given by equation 5.19 where  $\theta$  is the angle between the incident and scattered directions, *f* is the forward scattering factor, and *g*' is the asymmetry factor for the truncated phase function [31].

$$\Phi(\cos\theta) = 2f\delta(1-\cos\theta) + (1-f)(1+3g'\cos\theta)$$
(5.19)

Parameters f and g' are chosen such that the asymmetry factor matches that of the actual phase function determined via Mie theory, and the second moment matches that of the Henyey-Greenstein phase function. When used in conjunction with finite volume models, this method has been found to yield good agreement with calculations involving an exact phase function from Mie theory [28, 31, 32].

Absorption and scattering coefficients for a cloud of identically-sized spherical particles in the independent scattering regime are related to absorption and scattering efficiencies for a single particle by equations 5.20 and 5.21 where  $A_p$  is the geometric particle cross section,  $N_p$  is the number of particles per unit volume, and  $f_v$  is the particle volume fraction [28].

$$a_{\lambda} = A_p N_p Q_{abs,\lambda} = \frac{3}{2} \frac{f_v}{d_p} Q_{abs,\lambda}$$
(5.20)

$$\sigma_{\lambda} = A_p N_p Q_{sca,\lambda} = \frac{3}{2} \frac{f_v}{d_p} Q_{sca,\lambda}$$
(5.21)

As the finite volume technique utilized in this study does not explicitly account for spectral dependencies, the calculated spectral absorption efficiency, scattering efficiency and asymmetry factor are averaged over wavelength weighted by the blackbody intensity distribution at a given radiation temperature to achieve a spectrally averaged efficiency for a given radiation temperature. Radiation temperature is defined as the surface temperature of the emitting entity.

$$\overline{Q}_{avg}(T_{rad}) = \frac{\int_0^\infty Q(\lambda) I_{\lambda b}(\lambda, T_{rad}) d\lambda}{\int_0^\infty I_{\lambda b}(\lambda, T_{rad}) d\lambda}$$
(5.22)

The averages represented by equation 5.22 are computed numerically at a range of radiation temperatures external to the combined finite volume (FV) and computational fluid dynamics (CFD) simulation. Simple polynomial fits for spectrally averaged absorption efficiency, scattering efficiency, and asymmetry factor as a function of radiation temperature are input to the combined FV/CFD model with radiation temperature in control volume p determined via equation 5.23.

$$T_{rad,p} = \left(\frac{\int_{4\pi} I_p d\omega}{4\sigma}\right)^{1/4} \approx \left(\frac{\sum_{\ell} I_p^{\ell} \omega^{\ell}}{4\sigma}\right)^{1/4}$$
(5.23)

Volumetric absorption by steam present in the system is included via a weighted sum of gray gases (WSGG) approach in which a set of hypothetical gray gases is exploited to approximate a realistic non-gray gas [33]. The steam absorption coefficient is estimated by equations 5.24 and 5.25 in which  $a_i$  is the emissivity weighting factor for the  $i^{th}$  gray gas, T is the gas temperature,  $k_i$  is the absorption coefficienct for the  $i^{th}$  gray gas,  $p_{H2O}$  is the partial pressure of steam in the gas phase, s is the path length, and  $b_{ij}$  are the emissivity gas temperature polynomial coefficients.

$$a = -\frac{1}{s} \ln \left[ \sum_{i=0}^{I} a_i(T) \exp(-k_i p_{H_2O} s) \right]$$
(5.24)

$$a_i(T) = \sum_{j=1}^{J} b_{i,j} T^{j-1}$$
(5.25)

Coefficients are taken from Smith et al.[33] for both low pressure and atmospheric pressure water vapor with i = 3 and j = 4. The absorption coefficient *a* at a given steam partial pressure is determined from linear interpolation between the resulting low and high pressure values with

path length assumed equal to the tube radius. Absorption by  $CO_2$  is neglected owing to anticipated low  $CO_2$  partial pressure in regions with appreciable radiative intensity.

## 5.3.5 Optical properties

Surface optical properties utilized in both Monte Carlo and finite volume radiation models are summarized in Table 5.3. Data for the spectral complex index of refraction of Al, Ni and quartz is taken from Palik et al. [34]. Unpolished tube surfaces are treated as opaque and diffuse-gray whereas polished specularly reflective surfaces are assumed optically smooth with spectral directional optical properties employed in the Monte Carlo model and calculated from electromagnetic theory. The finite volume model applies only to energy emitted at relatively long wavelengths compared to those characterizing solar energy and, for the materials considered in this study, spectral variations are insignificant.

Material	Boundary	MC model properties (solar energy)	FV model properties (emitted energy)	
Cavity wall (Al)	Opaque, Specular	Spectral/directional from n,k	Uniform ( $\rho = 0.92, \epsilon = 0.08$ )	
Window cooling plate (Ni)	Opaque, Specular	Spectral/directional from n,k	Uniform ( $\rho = 0.87, \epsilon = 0.13$ )	
Window (SiO <sub>2</sub> )	Semi- transparent, Specular	Spectral/directional from n,k	Directional, $n = 1.5$ , $k = 0$	
Tubes (SiC)	Opaque, Diffuse	Uniform ( $\rho = 0.04, \epsilon = 0.96$ )	Uniform ( $\rho = 0.04, \epsilon = 0.96$ )	
Tubes (Inconel 600)	Opaque, Diffuse	Uniform ( $\rho = 0.20, \epsilon = 0.80$ )	Uniform ( $\rho = 0.20, \epsilon = 0.80$ )	

 Table 5.3: Summary of surface optical property inputs to Monte Carlo and finite volume radiation models

Figure 5.10 illustrates the spectral directional reflectivity for optically smooth aluminum and quartz surfaces calculated via equations 3.41 - 3.44. Significant spectral and directional variability is evident for polished aluminum (Figure 5.10a) with  $\lambda < 1 \mu m$ ; however, for  $\lambda > 1 \mu m$  spectral dependence becomes minimal and directional variability is only noteworthy as incident rays become tangential to the surface with large incident angles ( $\theta > 70^\circ$ ) relative to the surface normal.



Figure 5.10: Spectral directional reflectivity of (a) aluminum and (b) quartz

The fraction of energy emitted below 1  $\mu$ m is only 0.02, 0.04, and 0.07 for surface temperatures of 1600 K, 1800 K, and 2000 K respectively indicating that, for conditions of interest, the vast

majority of thermal emission occurs in a wavelength interval over which spectral variations are negligible. Literature data for polished aluminum indicates a normal spectral reflectivity in the range of 0.9 - 0.95 over a wavelength range of 1-8 µm [35]. The quartz surface in Figure 5.10(b) exhibits strongly directional reflectivity with little spectral variability over 0.5 - 7.5 µm arising from a nearly constant refractive index in this range. More than 90% of the emitted energy falls within this wavelength interval for any realistic surface temperature above 1300 K. Based on these observations, spectral variability for both aluminum and quartz surfaces is disregarded in the finite volume model for emitted energy, whereas directional variability is retained only for the quartz surface.

The average diameter reported for acetylene black particles investigated in this study (Chevron Phillips Chemical Company, Shawinigan Black®) is 42 nm. Spectral values of the complex index of refraction for the particle material are approximated as those for propane soot [36] and the corresponding spectral absorption efficiency, scattering efficiency, and scattering phase function calculated from Mie theory for a 42 nm particle diameter are shown in Figures 5.11 and 5.12. Small particle size permits estimation of Mie theory computations with a comparatively simple Rayleigh limit assessed via equations 5.26-5.28 assuming a nonparticipating fluid medium [28].

$$Q_{abs} = \frac{24\pi d_p}{\lambda} \frac{nk}{\left(n^2 - k^2 + 2\right)^2 + 4n^2k^2}$$
(5.26)

$$Q_{sca} = \frac{8}{3} \left(\frac{\pi d_p}{\lambda}\right)^4 \frac{\left[\left(n^2 - k^2 - 1\right)\left(n^2 - k^2 + 2\right) + 4n^2 k^2\right]^2 + 36n^2 k^2}{\left[\left(n^2 - k^2 + 2\right)^2 + 4n^2 k^2\right]^2}$$
(5.27)

$$\Phi = \frac{3}{4} \left( 1 + \cos^2 \theta \right) \tag{5.28}$$



Figure 5.11: Spectral absorption and scattering efficiency for 42 nm acetylene black particles



Figure 5.12: Spectral scattering phase function for 42 nm acetylene black particles

Absorption and scattering efficiencies from Mie theory agree with those calculated in the Rayleigh limit within 0.5% for  $\lambda > 0.7 \mu m$  or, correspondingly,  $\xi < 0.3$ . Carbon particles are not directly exposed to energy emitted in the solar spectrum and, for surface temperatures below 2000 K, at most 0.8% of blackbody emission occurs below 0.7  $\mu m$ . Thus the Rayleigh limit is highly accurate for more than 99% of the spectrum emitted by heated tube surfaces and provides a convenient explicit relationship between particle size and absorption or scattering efficiency

which can be exploited to assess the behavior of shrinking reactive particles. Figure 5.13 indicates that spectrally averaged absorption and scattering efficiency increase with radiation temperature due to a comparatively larger contribution from thermal emission at short wavelengths.



Figure 5.13: Spectrally averaged absorption and scattering efficiency as a function of radiation temperature

Volumetric absorption within the interior of the quartz window is computed using equation 5.29 [28] and the spectral extinction coefficient, k [34] whereas the spectral transmissivity,  $\tau_{\lambda}$ , is determined from the absorption coefficient and the path length l, in equation 5.30.

$$a_{\lambda} = \frac{4\pi k}{\lambda} \tag{5.29}$$

$$\tau_{\lambda} = \exp(-a_{\lambda}l) \tag{5.30}$$

Figure 5.14 illustrates the spectral absorption coefficient and transmissivity for the quartz window with a path length at normal incidence equal to the thickness of the receiver window (0.95 cm). Oblique incidence angles lengthen the path by which the radiative energy travels

through the window leading to slightly lower hemispherically averaged values. The absorption coefficient is uniformly zero over  $0.16 - 3.6 \mu m$  and thus, as more than 98.5% of the solar spectrum lies within this range, volumetric absorption of solar energy by the quartz window is inconsequential.



Figure 5.14: Spectral absorption coefficient and transmissivity for the quartz window

However, volumetric absorption cannot be discounted for the longer wavelengths characterizing energy emitted by heated surfaces within the receiver. The hemispherically averaged window transmissivity is weighted by the blackbody intensity distribution at a given emission temperature and spectrally averaged in a procedure analogous to that for absorption and scattering efficiency in equation 5.22. Spectrally averaged transmissivity is shown in Figure 5.15 along with an average absorption coefficient determined from equation 5.30. A single value of the absorption coefficient is selected for the combined FV/CFD model assuming emission at 1600 K. Active cooling of the quartz surface renders calculation results insensitive to the volumetric absorption coefficient because radiative energy is either transmitted through the window and lost directly, or internally absorbed by the quartz panel and dissipated via

conduction into receiver cooling zones. Thus the magnitude of the absorption coefficient controls the means by which energy is lost through the window, but not the quantity of energy removed from the interior of the receiver.



Figure 5.15: Spectrally averaged quartz transmissivity and absorption coefficient

# **5.4 Fluid Flow Models**

### 5.4.1 Dimensionless parameters and characteristic times

Dimensionless parameters and characteristic times associated with flow through each tube under typical receiver operating conditions are shown in Table 5.4 along with the Grashof number for buoyant flow in the cavity. All values are calculated for spherical carbon particles with a uniform diameter of 42 nm, consistent with the average diameter of acetylene black particles utilized in experiments. The nano-sized particles are characterized by momentum and thermal Stokes numbers well under  $10^{-4}$  implying equivalent fluid and particulate phase velocity and temperature.

••	-		
	Range of		
Parameter	values		
Re	<250		
St	$2x10^{-6} - 2x10^{-5}$		
$St_{th}$	2x10 <sup>-6</sup> - 9x10 <sup>-5</sup>		
Bi	$7x10^{-3} - 8x10^{-2}$		
$Bi_r$	4x10 <sup>-7</sup> - 1x10 <sup>-4</sup>		
Sc	$5x10^3 - 1x10^4$		
Ri	0.2 - 3.0		
$\tau_{conv}(s)$	8x10 <sup>-9</sup> - 1x10 <sup>-8</sup>		
$\tau_{rad}$ (s)	$1 x 10^{-3} - 4 x 10^{-5}$		
$\tau_{cond}$ (s)	5x10 <sup>-11</sup> - 3x10 <sup>-10</sup>		
$\tau_{flow}(s)$	0.2 - 1.2		
$Gr_{(cavity)}$	$5x10^4 - 8x10^6$		

 Table 5.4: Dimensionless parameters and characteristic times for typical operating conditions

Uniform internal particle temperature is justifiable based on the Biot number calculated in the case of either external convective heat transfer with the fluid (Bi), or radiative exchange with the tube wall ( $Bi_r$ ). The characteristic time for convection is at least three orders of magnitude smaller than that for radiation implying that particle and local gas phase temperatures equilibrate by convection more rapidly than particles are heated by radiation exchange with the tube wall. Relatively high values of the Schmidt number indicate minimal contribution of Brownian motion to particle transport and moderate values of the Richardson number imply equivalent importance of both natural and forced convective flow within the tubes. Both forced convection through the tubes and buoyant flow induced within the cavity space between the heated tube surfaces and the cooled cavity walls are laminar as indicated by the Reynolds and Grashof numbers, respectively. Appendix A provides corresponding values as a function of particle size and indicates that assumptions regarding uniform internal particle temperature and equivalent fluid and particulate

velocity and temperature are valid up to particle diameters on the order of 5-30  $\mu$ m, more than 100 times the nominal particle diameter. Thus particle aggregation is unlikely to invalidate the assumptions underlying the fluid flow model.

#### 5.4.2 Fluid flow model

Two-phase flow within the tubes can be described by an Eulerian-Eulerian two-fluid model in which the solid is treated as a quasi-continuous phase via temporal or statistical averaging procedures [37, 38]. Neglecting interfacial shear stress, the corresponding steady state mass and momentum transport equations for the  $k^{\text{th}}$  phase are given in equations 5.31 and 5.32 where  $\alpha_k$ ,  $\rho_k$ , and  $\vec{v}_k$  are, respectively, the volume fraction, density and velocity of the  $k^{\text{th}}$  phase, pis the pressure, and  $\vec{g}$  is the acceleration due to gravity.

$$\nabla \cdot \left( \alpha_k \rho_k \vec{\upsilon}_k \right) = \Gamma_k \tag{5.31}$$

$$\nabla \cdot \left(\alpha_k \rho_k \vec{\upsilon}_k \vec{\upsilon}_k\right) = -\alpha_k \nabla p_k + \nabla \cdot \left(\alpha_k \vec{\vec{\tau}}_k\right) + \alpha_k \rho_k \vec{g} + \vec{M}_{jk}$$
(5.32)

The stress tensor for the  $k^{\text{th}}$  phase  $(\vec{\tau}_k)$  is neglected for the solid as the assumption of dilute particle flow or low volume loading renders particle-particle contact improbable. For the fluid phase, the gases are assumed ideal and the corresponding stress tensor is provided by equation 5.33 where  $\mu_g$  is the viscosity of the fluid phase.

$$\vec{\tilde{\tau}}_{g} = \mu_{g} \left[ \left( \nabla \vec{\upsilon}_{g} + \nabla \vec{\upsilon}_{g}^{T} \right) - \frac{2}{3} \nabla \cdot \vec{\upsilon}_{g} I \right]$$
(5.33)

Two-way coupling between phases is included via interphase transport terms  $\Gamma_k$  and  $M_{jk}$ . Neglecting virtual mass and Bassett forces, the interphase gas-particle momentum transport term  $M_{gp}$  is given in equation 5.34 for drag in the Stokes regime.

142

$$M_{gp} = -M_{pg} = \frac{18\alpha_{p}\mu_{g}}{d_{p}^{2}C_{c}} \left(\vec{v}_{p} - \vec{v}_{g}\right)$$
(5.34)

For a Stokes number well under unity it can be shown that the difference between the particle and gas phase velocity is negligible [37-39] and for a well dispersed particle phase with low particle volume loading the individual phase mass and momentum transport equations can be combined through addition to yield single fluid mixture equations.

$$\nabla \cdot (\rho \vec{v}) = 0 \tag{5.35}$$

$$\nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\alpha_g \vec{\tilde{\tau}}_g) + \rho \vec{g}$$
(5.36)

$$\rho = \alpha_g \rho_g + \alpha_p \rho_p \approx \frac{\rho_g}{1 - w_p}$$
(5.37)

The single fluid mixture model treats the two-phase mixture as a single fluid described by a volume averaged density,  $\rho$ . In equations 5.35-5.37  $\vec{v}$  is the velocity of both fluid and particulate phases, and  $w_i$  is the mass fraction of the  $i^{\text{th}}$  phase. Although particle volume loading is minimal, the corresponding particle mass loading may be considerable due to the disparity between fluid and solid densities.

Neglecting viscous dissipation, diffusional energy sources, and kinetic energy terms the energy equation for phase k is given by equation 5.38 and 5.39 [37-40].

$$\nabla \cdot (\alpha_k \rho_k \vec{\upsilon}_k h_k) = \nabla \cdot (\alpha_k k_k \nabla T_k) + S_k + Q_{ik}$$
(5.38)

$$h_k = \sum_c w_c \int_{T_{ref}}^T Cp_c dT$$
(5.39)

Thermal conductivity of the  $k^{th}$  phase is denoted by  $k_k$ ,  $S_k$  is an energy source term for the  $k^{th}$  phase, and the enthalpy of phase k ( $h_k$ ) is determined from a mass-weighted summation over constituent species. Solid phase conduction is neglected as particle-particle contact is highly

improbable under conditions of low volume loading. Energy transport between phases is denoted by  $Q_{ik}$  and expressed by equation 5.40 for spherical particle with negligible slip velocity and diameter  $d_p$ .

$$Q_{gp} = -Q_{pg} = \frac{6\alpha_{p}h_{pg}}{d_{p}} \left(T_{p} - T_{g}\right)$$
(5.40)

For a particle thermal Stokes number well under unity, the difference between fluid and particle phase temperatures may be neglected and an overall mixture energy equation is derived by summation of individual phase equations [37-39]. Mixture heat capacity can be described by equation 5.42 and is approximately equal to a mass-weighted average.

$$\nabla \cdot (\rho \vec{v} h) = \nabla \cdot (\alpha_g k_g \nabla T_g) + S \tag{5.41}$$

$$\rho Cp = \alpha_g \rho_g Cp_g + \alpha_p \rho_p Cp_p \approx \rho \left( w_g Cp_g + w_p Cp_p \right)$$
(5.42)

The steady state transport equation describing individual species mass fraction for each fluid species in the mixture is given by equation 5.43 in which  $D_i$  are binary diffusion coefficients for the *i*<sup>th</sup> species in the mixture and the source term  $S_i$  results from reactions involving species *i* [40].

$$\nabla \cdot \left(\rho \vec{\upsilon} w_i\right) = \nabla \cdot \left(\rho D_i \nabla w_i\right) + S_i \tag{5.43}$$

The steady state population balance for an aerosol particulate phase is expressed in equation 5.44 where  $\hat{n}_p$  is the mass-based particle number concentration,  $D_p$  is the Brownian diffusion coefficient, and  $\vec{C}_{th}$  is the thermophoretic velocity arising from temperature gradients in the system [41, 42].

$$\nabla \cdot \left(\rho \vec{\upsilon} \hat{n}_{p}\right) = \nabla \cdot \left(\rho D_{p} \nabla \hat{n}_{p}\right) - \nabla \cdot \left(\rho \vec{C}_{th} \hat{n}_{p}\right)$$
(5.44)

For particles characterized by a diameter less than the mean free path of the gas, the thermophoretic velocity may be approximately determined from equation 5.45 [43].

$$\vec{C}_{th} = \frac{-0.55\,\mu_g}{\rho T} \nabla T \tag{5.45}$$

## 5.4.3 Fluid properties

The single fluid mixture model defined by equation 5.35-5.37, and 5.41-5.45 adequately describes the two-phase flow within the receiver. Gas viscosity and binary mixture diffusivities at elevated temperatures are estimated via Chapman-Enskog theory [40] for non-polar molecules, whereas thermal conductivity of gases are assessed from either Chapman-Enskog theory for monatomic gases or from a modified Eucken correlation for polyatomic molecules [44] and compared with literature data where available. The Chapman-Enskog models are given by equations 5.46 and 5.47 in which  $\sigma_c$  is the collision diameter and  $\Omega$  is the collision integral [40].

$$\mu = 2.6693 \times 10^{-6} \, \frac{\sqrt{MT}}{\sigma_c^2 \Omega_{\mu}} \tag{5.46}$$

$$k = 0.0833 \frac{\sqrt{T/M}}{\sigma_c^2 \Omega_k} \tag{5.47}$$

The modified Eucken correlation is given by equation 5.48 where  $C_p$  is the molar heat capacity of the gas species.

$$k = \left(1.32\frac{C_p}{M} + 0.88\frac{R}{M}\right)\mu\tag{5.48}$$

Viscosity and thermal conductivity of gas mixtures are determined from their constituent species using a semi-empirical formula given by Bird et al. where  $x_i$  is the mole fraction of species *i* in the fluid mixture [40].

$$\mu_{g} = \sum_{i=1}^{N_{g}} \frac{x_{i} \mu_{i}}{\sum_{j} x_{j} \Phi_{ij}}$$
(5.49)

$$\Phi_{ij} = \frac{1}{\sqrt{8}} \left( 1 + \frac{M_i}{M_j} \right)^{-\frac{1}{2}} \left[ 1 + \left( \frac{\mu_i}{\mu_j} \right)^{\frac{1}{2}} \left( \frac{M_j}{M_i} \right)^{\frac{1}{4}} \right]^2$$
(5.50)

The mass diffusivity of each gas component in argon is estimated in a dilute approximation using either Chapman-Enskog theory or the correlation from Fuller et al. [45]. All calculated viscosity, thermal conductivity, and binary diffusivity values agree with literature data available up to temperatures in the range of 700-800 K as shown in Appendix B [46-49]. The Brownian diffusion coefficient for the aerosol phase in equation 5.44 is provided by equation 5.51 where  $k_B$ is the Boltzmann constant, and  $C_c$  is the Cunningham correction factor accounting for slip at the particle surface [43].

$$D_p = \frac{k_B T C_c}{3\pi\mu_g d_p} \tag{5.51}$$

For particles with a diameter less than 100 nm the correction factor can be approximated by equation 5.52 [43].

$$C_{c} = 1 + \frac{\lambda}{d_{p}} \left[ 2.514 + 0.8 \exp\left(-0.55\frac{d_{p}}{\lambda}\right) \right]$$
(5.52)

Though diffusivity of 42 nm carbon particles is on the order of  $10^{-8}$  m<sup>2</sup>/s and, correspondingly, the magnitude of the Schmidt number implies negligible contribution from Brownian motion compared to convective fluid flow, the diffusion term in equation 5.44 is retained for reasons of numerical stability [42]. The gas mean free path,  $\lambda$ , is given by equation 5.53 where  $d_m$  is the collision diameter for the constituent gas molecules.

$$\lambda = \frac{k_B T}{\sqrt{2\pi d_m^2 p}} \tag{5.53}$$

## 5.5 Reaction models

### 5.5.1 Reaction processes and equilibrium compositions

The primary process of interest is the heterogeneous endothermic carbon-steam gasification reaction at the acetylene black particle surface given in equation 5.54 though, at relevant conditions, the homogeneous water gas shift reaction in equation 5.55 cannot be ignored.

$$C_{(s)} + H_2 O_{(g)} \to CO_{(g)} + H_{2(g)} \qquad \Delta H_r^0 = 131.3 \text{ kJ/mol}$$
 (5.54)

$$CO_{(g)} + H_2O_{(g)} \leftrightarrow CO_{2(g)} + H_{2(g)} \quad \Delta H_r^0 = -40.8 \text{ kJ/mol}$$
(5.55)

In theory both the endothermic Boudouard and slightly exothermic hydrogasification reactions provided in equations 5.56 and 5.57 are possible.

$$C_{(s)} + CO_{2(g)} \rightarrow 2CO_{(g)} \quad \Delta H_r^0 = 172.5 \ kJ/mol$$
 (5.56)

$$C_{(s)} + 2H_{2(g)} \rightarrow CH_{4(g)} \Delta H_r^0 = -74.9 \, kJ/mol$$
 (5.57)

However, the Boudouard reaction is neglected as the rate is typically three to four times slower than that for steam gasification at typical gasifier conditions [50-52], and  $CO_2$  is only produced by the water-gas shift reaction in relatively small quantities in the coolest regions of the tube. Hydrogasfication is generally several orders of magnitude slower than steam gasification [51, 52] and thus is also disregarded. Figure 5.16 shows equilibrium compositions produced from an initial equimolar carbon/steam mixture at atmospheric pressure evaluated using FactSage thermodynamic software [53]. The steam gasification reaction is thermodynamically projected to proceed to completion at temperatures above 1100-1200 K while formation of  $CO_2$  and  $CH_4$  is only thermodynamically favored below 900 K.



Figure 5.16: Equilibrium compositions for an initially equimolar carbon/steam mixture at atmospheric pressure

## 5.5.2 Surface reaction mechanism for steam gasification

The carbon-steam surface reaction is typically presumed to follow either an oxygenexchange or hydrogen inhibition mechanism. The oxygen-exchange mechanism consists of dissociative reversible adsorption of  $H_2O$  on the carbon surface followed by irreversible combination of adsorbed oxygen atoms with surface carbon [23, 51, 54-58]. The hydrogen inhibition mechanism, on the other hand, is based on irreversible dissociative  $H_2O$  adsorption, reversible  $H_2$  adsorption, and irreversible combination of adsorbed oxygen atoms with surface carbon [23, 54]. Though the origin of hydrogen inhibition differs in each mechanism, both lead to an identical Langmuir-Hinshelwood rate expression shown in equation 5.58 with kinetic parameters provided by a conventional Arrhenius expression in equation 5.59.

$$r_{c} = \frac{k_{1}p_{H_{2}O}}{1 + \frac{1}{k_{2}}\left(k_{1}p_{H_{2}O} + k_{-1}p_{H_{2}}\right)}$$
(5.58)

$$k_i = k_{i0} \exp\left(-\frac{E_a}{RT}\right) \tag{5.59}$$

Many other mechanisms have been proposed in the literature [51, 59] including those applicable for combined  $CO_2/H_2O$  gasification [56] or gasification at elevated pressures [60].

At low partial pressures the effect of hydrogen inhibition is frequently neglected such that the Langmuir-Hinshelwood rate expression can be condensed into a simple n<sup>th</sup> order global model of the form shown in equation 5.60 [23, 51].

$$r_c = k' p_{H_2O}^n (5.60)$$

Given the inherent complexity of radiative and convective/conductive heat transfer models detailed above, it is advantageous to simplify the reaction model as much as possible while retaining sufficient detail to capture a reasonably realistic depiction of the chemical process. Figure 5.17 provides a comparison between the reaction rate predicted by the full Langmuir-Hinshelwood (L-H) rate expression and that estimated from a simplified 1<sup>st</sup> order model with kinetic parameters from Muhlen et al. [56].



Figure 5.17: Steam gasification reaction rate predicted by a full Langmuir Hinshelwood kinetic expression and a simplified first order model

The variable  $P_{H2O,initial}$  refers to steam partial pressure at 0% conversion. The first order model closely approximates the rate predicted by the full Langmuir-Hinshelwood expression at both

high temperature and high conversion implying minimal impact of hydrogen inhibition. Errors in the approximate first order rate expression may be substantial at either low temperature (<1200 K) or a combination of high steam partial pressure and low conversion at high temperature. However, the low temperature condition is not of interest for the current study and the combination of high temperature with high steam partial pressure and low conversion is unlikely to transpire. Thus inhibition is neglected in the current study and a simple first order rate expression is applied in the computational model.

### 5.5.3 Particle reaction model

A progressive conversion scheme provides a macroscopic description of the heterogeneous surface reaction occurring within the entirety of the porous particle. The overall particle reactivity on a surface area basis is described by equation 5.61 for a first order reaction.

$$R_s = \eta k_s P_{H_2O_s} \tag{5.61}$$

In equation 5.61  $R_s$  is the surface reaction rate,  $k_s$  is the intrinsic first order reaction rate constant on an area basis,  $P_{H_2O_s}$  is the partial pressure of steam at the external particle surface and, in the absence of external mass transfer limitations, can be set equal to the local bulk partial pressure of steam in the fluid phase. The effectiveness factor  $\eta$  is derived from local steam concentration profiles within the spherical particle determined from a steady state mass balance given by equations 5.62-5.64 under the assumptions of uniform internal particle temperature, an irreversible first order rate expression, dilute gaseous reactant species, and negligible external mass transfer limitations [51].

$$\frac{1}{r^2} \frac{d}{dr} \left( r^2 D_e \frac{dC_{H2O}}{dr} \right) - k_s \hat{A}_s \rho_p C_{H2O} = 0$$
(5.62)

$$C_{H2O} = C_{H2O,s}$$
 at  $r = R_p$  (5.63)

$$\frac{dC_{H2O}}{dr} = 0$$
 at  $r = 0$  (5.64)

In equation 5.62  $\hat{A}_s$  is the specific internal surface area of the particle on a mass basis,  $\rho_p$  is the particle density, and  $C_{H2O,s}$  is the steam concentration at the external surface of the particle. The effective diffusivity  $(D_e)$  for the gaseous reactant species within the pores is approximated by equation 5.65 where  $\psi$  is the particle porosity, D is the binary diffusion coefficient in the bulk fluid, and  $\tau$  is the pore tortuosity frequently prescribed a value of  $\sqrt{2}$ .

$$D_e = \frac{D\psi}{\tau^2} \tag{5.65}$$

Assuming uniform internal temperature, equations 5.62-5.65 can be solved analytically within the interior of the particle [51, 61] yielding equation 5.66 with the Thiele modulus defined in equation 5.67.

$$\frac{C_{H2O}}{C_{H2O_s}} = \frac{R_p}{r} \frac{\sinh\left(\phi \frac{r}{R_p}\right)}{\sinh(\phi)}$$
(5.66)

$$\phi = R_p \left(\frac{k_s \hat{A}_s \rho_p}{D_e}\right)^{1/2} \tag{5.67}$$

The effectiveness factor is taken to be the ratio of the actual overall rate to the rate if the entire internal particle surface was exposed to the external surface concentration  $C_{H2O,s}$ , and is derived in equation 5.68.

$$\eta = \frac{\overline{C}_{H2O}}{C_{H2O,s}} = \frac{\int_{0}^{R_{p}} \frac{C_{H2O}}{C_{H2O,s}} r^{2} dr}{\int_{0}^{R_{p}} r^{2} dr} = \frac{3}{\phi} \left(\frac{1}{\tanh\phi} - \frac{1}{\phi}\right)$$
(5.68)

#### 5.5.4 Global reaction model

The global volumetric reactivity required for the computational fluid dynamics (CFD) model can be determined from the intrinsic surface reactivity via equation 5.69 assuming that the surface reaction follows a progressive conversion scheme.

$$R_{v} = R_{s}\hat{A}_{s}w_{c}\rho = \eta k_{s}P_{H2O,s}\hat{A}_{s}w_{c}\rho$$
(5.69)

In equation 5.69  $\hat{A}_s$  is the specific surface area of the particle on a mass basis,  $w_c$  is the weight fraction of carbon in the two-phase mixture, and  $\rho$  is the mixture density provided by equation 5.37. The product of the first two terms represents the reaction rate per particle mass whereas the product of the last two terms represents the particle mass per unit total volume. For ease of input into the CFD model the global volumetric reaction rate given in equation 5.69 is recast in terms of steam and carbon molar concentrations in equation 5.70 where *R* is the gas constant, *T* is the local temperature, and  $M_c$  is the molecular weight of carbon.

$$R_{v} = \eta k_{s} R T \hat{A}_{s} M_{c} C'_{H20} C'_{c}$$
(5.70)

Though both internal and external particle specific surface area vary as the reaction progresses, attempts to correlate reactivity of coal char to specific surface area as a function of reaction conversion have generally been unsuccessful [51]. Detailed studies of the specific surface area of coal chars during gasification indicate that, at low conversion, micropores are opened and new pore connections are formed as the reaction proceeds leading to an increase in specific surface area with conversion. After this initial period, the trend reverses and a decrease in specific surface area with reactant conversion is noted due to pore wall destruction and pore merging [51, 62, 63]. For the purposes of this study a simple constant specific surface area is assumed given a lack of detailed information regarding pore structure and surface area development for the

acetylene black particles. The magnitude of the specific surface area is taken as the initial value  $(75 \text{ m}^2/\text{g})$  provided by the supplier. Modifications to this constant value are considered in the framework of a sensitivity analysis detailed in subsequent sections.

Particles in this study are characterized by  $d_p = 42$  nm,  $\rho = 1750$  kg/m<sup>3</sup> and  $\hat{A}_s = 75$  m<sup>2</sup>/g. The effectiveness factor is greater than 0.999 implying negligible internal mass transfer limitations for temperatures up to 2000 K and porosity as low as 0.01 with kinetic parameters from Trommer et al. [64]. Calculations of the effectiveness factor as a function of particle diameter are provided in Appendix A. For a particle size of 1 µm the effectiveness factor is greater than 0.995 for temperatures up to 2000 K and porosity greater than 0.1. Both particle size and density may exhibit complex dependence on reaction conversion. At one extreme all reaction occurs at the external surface and the particles decrease in size while retaining constant density, whereas at the other extreme reaction occurs entirely within the interior and particles maintain constant size with decreasing density. When reaction occurs exclusively on the external surface the particle diameter can be related to the initial particle diameter ( $d_{p0}$ ) and the reaction conversion (X) by a shrinking particle model in equation 5.71.

$$d_{p} = d_{p0} (1 - X)^{1/3} \tag{5.71}$$

Conversion is determined from local variables in the CFD model adjusted for gas expansion and generation by the heterogeneous surface reaction [61] via equation 5.72 under the assumption of a uniformly well-dispersed particle phase.

$$(1-X) = \frac{w_c \rho}{w_{c,0} \rho_0} \frac{T}{T_0} \frac{P_0}{P} \left( 1 + \xi X \frac{n_{c0}}{n_{f0}} \right)$$
(5.72)

In equation 5.72  $w_c$  is the weight fraction of carbon particles and  $\rho$  is the mixture density with  $w_{c0}$  and  $\rho_0$  referring to conditions at the tube inlet,  $\xi$  is the number of moles gas generated per

mole of solid reacted,  $n_{c0}$  is the molar flow rate of carbon at the tube inlet, and  $n_{f0}$  is the fluid molar flow rate at the tube inlet. Despite negligible particle diffusion by Brownian motion, thermophoretic movement in response to temperature gradients produces carbon profiles which violate the assumption of uniform dispersion. Thus the expression in equation 5.72 overestimates conversion for hot regions in which particle concentration is diminished by thermophoresis even in the absence of reaction. A more accurate expression for conversion requires a detailed history for each particle, information which is not available from the models considered in this study.

Provided particle diameter never exceeds a value for which assumptions underlying the single fluid mixture model are violated, particle size only impacts the solution via particle diffusivity and absorption or scattering parameters. Absorption and scattering parameters can be approximated in the Rayleigh limit and thus the combination of equations 5.20 and 5.26 implies that the absorption coefficient is independent of particle size. Though scattering of radiative energy is heavily dependent on particle diameter, the relative magnitudes of absorption and scattering efficiencies in Figure 5.11 indicate that the extinction coefficient for acetylene black particles is unquestionably dominated by absorption. Brownian diffusivity of the unreacted particles is negligible and retained only to enhance numerical stability. Calculations of the Schmidt number as a function of particle diameter in Appendix A indicate that Brownian diffusion is not likely to become physically relevant until the particles shrink to less than 40% of their original size. Equation 5.71 dictates that over 90% of the particle mass must be converted before the particle shrinks to 40% of its original diameter, even assuming reaction occurs exclusively on the external surface. Thus sensitivity of simulation results to particle diameter should be minimal and, for simplicity, a constant particle diameter is applied in the calculations.

### 5.5.5 Water gas shift reaction

Forward and reverse water gas shift reactions are described by equation 5.55 and included via two separate homogeneous gas phase reactions. Rate expressions for the uncatalyzed water gas shift reactions are typically treated as first order in all gas components [65-67], though some authors describe the reactions as half-order in terms of both CO and  $H_2$  [68, 69]. The rate expressions for each the forward and reverse reaction are described by equations 5.73 and 5.74 assuming first order dependence.

$$R_{f} = k_{f} C_{CO} C_{H2O}$$
(5.73)

$$R_b = k_b C'_{H2} C'_{C02} \tag{5.74}$$

Arrhenius parameters for the forward rate constant were taken from the literature [66] whereas the rate constant for the reverse reaction were calculated from the forward rate constant and the equilibrium constant determined using FactSage thermodynamic software [53] via equation 5.75.

$$k_b = \frac{k_f}{K_{eq}} \tag{5.75}$$

## 5.6 Combination and solution of radiation, fluid flow, and reaction models

Approximate solutions for the system of coupled differential equations, including the finite volume model for emitted radiative energy, are obtained via the commercial computational fluid dynamics software ANSYS FLUENT version 6.3.26. The computational fluid flow and reaction models are solved simultaneously and on the same spatial mesh as the finite volume model for emitted radiation leading to close coupling between temperature profiles and radiative energy solutions. The net rate of radiative energy supplied to a control volume is given by the

negative of the divergence of the radiative flux vector in equation 5.77 and added to the right hand side of the energy equation [28].

$$\vec{q}_r = \int_{0}^{4\pi} I(\theta, \varphi) \vec{s} \, d\omega \tag{5.76}$$

$$-\nabla \cdot \vec{q}_{r} = -\int_{0}^{4\pi} \frac{dI}{dS} d\omega = a \int_{0}^{4\pi} I(\theta, \varphi) d\omega - 4\pi a I_{b}$$
(5.77)

The variable *S* is the coordinate along the path ( $\vec{s}$ ) traveled by the radiant energy, *a* is the absorption coefficient, and *I*<sub>b</sub> is the blackbody intensity given by equation 5.78.

$$I_b = \frac{\sigma}{\pi} T^4 \tag{5.78}$$

The divergence of the radiative flux vector and thus the volumetric radiative energy source term reduce to zero in the absence of absorption, regardless of scattering behavior. In the finite volume scheme the integral in equation 5.77 is replaced by a finite summation over solid angles  $\omega^{l}$ .

$$-\nabla \cdot \vec{q}_r = a \sum_{\ell} I^{\ell} \omega^{\ell} - 4\pi a I_b$$
(5.79)

Spatial profiles of solar energy absorbed along each surface in the receiver are determined external to the CFD model via the Monte Carlo technique detailed in Chapter 3 and section 5.3 and subsequently input into the CFD model by means of an energy generation function across a thin slice of each solid surface. The thickness of the slice is maintained at a fixed value of  $10^{-5}$  m as absorption is predominantly a surface phenomenon. Each profile is generated with a set number of points containing global (*x*,*y*,*z*) position along with absorbed solar flux, and a zero-order interpolation scheme is employed to estimate flux values at the global position describing the centroid of each boundary mesh face in the CFD model. In order to validate this technique, a CFD model was solved with finite volume solutions for both the solar and emitted components.

A gray band model was utilized to separate the radiative energy into two components with an artificially small wavelength interval (0-0.01  $\mu$ m) stipulated for the solar energy in order to eliminate spectral overlap. Resulting profiles of absorbed solar flux were converted to energy generation functions across a thin slice of each solid surface, and input to a second CFD model accompanied by a single-band finite volume model for emitted energy. Both models produced identical solutions.

## 5.6.1 Boundary conditions, discretization schemes, and convergence criteria

The computational fluid dynamics model is solved in only half of the receiver taking advantage of the geometric symmetry of the center line in order to enhance computational efficiency. However, the off-axis design of the High Flux Solar Furnace produces a slightly asymmetric solar flux profile thereby precluding exact validity of the symmetry assumption and, for this reason, the Monte Carlo model is solved within both halves of the receiver. Conversely the CFD model only utilizes profiles of solar energy absorbed within the comparatively hotter east half of the receiver and assumes symmetry in the temperatures achieved on the opposing side. As realistic tube temperatures on the west side are lower than those stipulated by symmetry, this simplification leads to slightly overestimated radiative intensity originating from emission by heated surfaces on the west side and, correspondingly, slightly overestimated east side temperatures.

The aerosol population balance is incorporated in the CFD model by means of a userdefined scalar transport equation for the particle weight fraction with combined thermophoretic diffusion and convective transport terms and a volumetric source to account for the gasification reaction. Carbon mass fraction is fixed to the user-defined scalar value for all points within the solution domain at each iteration. User-defined property definitions are also applied for gas viscosity, mixture thermal conductivity, mixture density, particle diffusivity, absorption coefficient, scattering coefficient, scattering phase function, and reaction conversion defined by equations 5.20-5.27, 5.37, 5.46-5.51, and 5.72.

A fully developed laminar flow profile at 300 K with uniform species and particle mass fractions is applied to each tube inlet. The flow profile is specified by means of mass flux via equation 5.80 with total mass flow rate (w) calculated from the sum of individual component flow rates.

$$\rho \upsilon = \frac{2w}{\pi R^2} \left( 1 - \frac{r^2}{R^2} \right)$$
(5.80)

A constant atmospheric tube outlet pressure is stipulated and all other variables at outflow boundaries are extrapolated from the interior solution domain. All external walls adjacent to cooling zones are fixed at a constant temperature of 300 K. A standard no-slip boundary condition with zero diffusive flux of all fluid species is imposed at walls adjacent to a fluid domain while particle concentration at solid surfaces is set to zero under the assumption that particles stick to and deposit on tube walls. Boundary conditions for the finite volume radiation model are enumerated in equations 5.6 - 5.10 and Table 5.3.

Scalar values at control volume faces are assessed from the surrounding nodal values using a second-order upwind discretization scheme so as to minimize false diffusion effects in the control-volume based approach employed by the CFD model. Facial values are determined via a Taylor series expansion about the upwind cell centroid shown in equation 5.81.

$$\varphi_f = \varphi + \nabla \varphi \cdot \vec{r} \tag{5.81}$$

Both nodal values and the gradients of the scalar ( $\varphi$ ) are evaluated at the centroid of the upwind control volume and  $\vec{r}$  represents the vector between the upwind cell and face centroids.

Gradients are approximated from surrounding nodal values through a Green-Gauss node based evaluation. Convergence is monitored by means of residual values representing a scaled imbalance between the left and right sides of the discretized transport equation. Additional monitors are placed on maximum tube temperatures, average tube temperatures at the horizontal center plane of the receiver, CO and  $CO_2$  molar flow at the tube outlets, and radiative energy absorbed by each tube. Convergence is judged by both the relative drop in scaled residuals from their initial values and the relative change in each surface and volume monitor between iterations. Converged solutions are typically obtained after residuals associated with momentum and continuity equations dropped three to four orders of magnitude whereas scaled residuals associated with energy and finite volume equations attained values on the order of  $10^{-8}$ - $10^{-7}$  in converged solutions.

## 5.7 Results and Discussion

## 5.7.1 Physical properties and model input parameters

Tables 5.5 – 5.9 provide the numerical constants or approximate polynomial temperature dependence of fluid properties, carbon particle properties, and solid properties. Polynomials are fit to Chapman-Enskog or modified Eucken models for fluid properties and literature data for solid properties [46-48, 70] over limited temperature ranges for ease of input into the CFD model. Silicon carbide properties are those reported for Hexoloy<sup>®</sup> SA SiC. All polynomials are limited such that realistic values are ensured over the entire temperature range attained during simulations. Carbon particle properties are reported by the supplier (Chevron Phillips Chemical Company, Shawinigan Black<sup>®</sup>) and absorption or scattering parameters are polynomial fits to the spectrally averaged values weighted by blackbody intensity illustrated in Figure 5.13.
Surface optical properties utilized in both Monte Carlo and finite volume radiation models are detailed in Table 5.3. Parameters describing the carbon-steam gasification and water-gas shift reactions are taken from the literature [64, 66] and the equation describing the temperature dependent water-gas shift equilibrium constant is fit to data generated by FactSage thermodynamic software [53].

R	8.314 J/mol/K
sigma	$5.6704 x 10^{-8} W/m^2/K^4$
$k_B$	1.38065x10 <sup>-23</sup> kg m <sup>2</sup> /s <sup>2</sup> /K
$MW_C$	12.011 g/mol
$MW_{CO}$	28.01 g/mol
$MW_{H2}$	2.02 g/mol
MW <sub>H2O</sub>	18.02 g/mol
$MW_{CO2}$	44.01 g/mol
$MW_{Ar}$	39.948 g/mol
$d_m$	$3.42 \times 10^{-10} \text{ m}$

Table 5.5: Simulation input parameters: constants

Table 5.6: Simulation input parameters: solid properties

$ ho_{SiC}$	3100 kg/m <sup>3</sup>	
$ ho_{Inconel}$	8470 kg/m <sup>3</sup>	
$ ho_{Al}$	$2702 \text{ kg/m}^3$	
$ ho_{quartz}$	2648 kg/m <sup>3</sup>	
$\rho_{Cu}$	8920 kg/m <sup>3</sup>	
$a_{quartz}$	$0.327 \text{ cm}^{-1}$	
n <sub>quartz</sub>	1.54	
k <sub>SiC</sub>	$\frac{185.7 - 0.314T + 3.05x10^{-4}T^{2} - 1.41x10^{-7}T^{3} + 2.60x10^{-11}T^{4} W/m/K}{59.4 W/m/K}$	$300 \text{ K} \le T \le 1600 \text{ K}$ T > 1600  K
k <sub>Inconel</sub>	$10.89 + 0.0123T + 2.98 \times 10^{-6} T^2 W/m/K$	300 K <u>≤</u> <i>T</i> <u>≤</u> 1500 K
$k_{Al}$	$235.4 + 0.0358T - 7.13x10^{-5}T^2 W/m/K$	300 K ≤ <i>T</i> ≤ 900 K
$k_{quartz}$	$0.260 + 5.49 \times 10^{-3} \text{T} - 7.72 \times 10^{-6} \text{T}^2 + 4.80 \times 10^{-9} \text{T}^3 \text{ W/m/K}$	300 K <u>≤</u> <i>T</i> <u>≤</u> 1200 K
$k_{Cu}$	421.2 - 0.0651T W/m/K	300 K <u>≤</u> <i>T</i> <u>≤</u> 1350 K
$Cp_{SiC}$	$251.1 + 2.03T - 1.72x10^{-3}T^{2} + 7.31x10^{-7}T^{3} - 1.19x10^{-10}T^{4}$ J/kg/K	$300 \text{ K} \le T \le 2200 \text{ K}$
$Cp_{Inconel}$	$385.7 + 0.202T + 7.40x10^{-6}T^2 J/kg/K$	300 K <u>≤</u> <i>T</i> <u>≤</u> 1500 K
$Cp_{Al}$	736.1 + 0.463T J/kg/K	300 K <u>≤</u> <i>T</i> <u>≤</u> 900 K
$Cp_{quartz}$	$-99.33 + 4.18T - 5.40x10^{-3}T^2 + 2.80x10^{-6}T^3$ J/kg/K	300 K <u>≤</u> <i>T</i> <u>≤</u> 847 K
$Cp_{Cu}$	$307.1 + 0.363T - 4.16x10^{-4}T^2 + 1.95x10^{-7}T^3 J/kg/K$	300 K <u>≤</u> <i>T</i> <u>≤</u> 1350 K

$dp_0$	42 nm	
$ ho_s$	$1750 \text{ kg/m}^3$	
$A_s$	75 m <sup>2</sup> /g	
$k_s$	$12.89 - 0.0346T + 4.06x10^{-5}T^2 - 2.12x10^{-8}T^3 + 4.05x10^{-12}T^4  W/m/K$	$300 \text{ K} \le T \le 2000 \text{ K}$
$Cp_s$	-615.2 + 5.81T - 5.34x10 <sup>-3</sup> T <sup>2</sup> + 2.33x10 <sup>-6</sup> T <sup>3</sup> - 3.90x10 <sup>-10</sup> T <sup>4</sup> J/kg/K 2043 J/kg/K	$300 \text{ K} \le T \le 2000 \text{ K}$ T > 2000  K
$Q_{abs}$	$(d_p/d_{p0})(-9.16x10^{-3}+5.11x10^{-5}T_{rad}-4.37x10^{-9}T_{rad}^2)$	$300 \text{ K} \le T_{rad} \le 2200 \text{ K}$
$Q_{sca}$	$(d_p^4/d_{p0}^4)(9.38x10^{-6} - 3.06x10^{-8}T_{rad} + 2.53x10^{-11}T_{rad}^2)$	$300 \text{ K} \le T_{rad} \le 2200 \text{ K}$

Table 5.7: Simulation input parameters: carbon particle properties

Table 5.8: Simulation input parameters: fluid properties (300 K < T < 2200 K)

$6.81 \times 10^{-6} + 4.00 \times 10^{-8} \text{T} - 5.47 \times 10^{-12} \text{T}^2 \text{ kg/m/s}$
$4.25 \times 10^{-6} + 1.75 \times 10^{-8} \text{T} - 2.08 \times 10^{-12} \text{T}^2 \text{ kg/m/s}$
$-4.13x10^{-6} + 4.580x10^{-8}T - 4.30x10^{-12}T^2 kg/m/s$
$6.46x10^{-6} + 3.53x10^{-8}T - 4.12x10^{-12}T^2 kg/m/s$
$9.76 x 10^{-6} + 4.96 x 10^{-8} T$ - $5.31 x 10^{-12} T^2 kg/m/s$
$7.74x10^{-6} + 3.70x10^{-8}T - 2.94x10^{-12}T^2 kg/m/s$
$8.31 x 10^{-3} + 6.47 x 10^{-5} T - 3.74 x 10^{-9} T^2 W/m/K$
$8.34x10^{-2} + 3.62x10^{-4}T - 1.59x10^{-8}T^2$ W/m/K
$-1.15 \times 10^{-2} + 1.08 \times 10^{-4} \text{T} + 1.09 \times 10^{-8} \text{T}^2 \text{ W/m/K}$
$1.64x10^{-3} + 6.45x10^{-5}T - 3.05x10^{-9}T^2 W/m/K$
$7.46 \times 10^{-3} + 3.19 \times 10^{-5} \text{T} - 4.35 \times 10^{-9} \text{T}^2 \text{ W/m/K}$
$-2.00x10^{-3} + 1.12x10^{-4}T - 6.32x10^{-8}T^2 + 2.13x10^{-11}T^3$ W/m/K
$977.1 + 0.234T - 6.49x10^{-5}T^{2} + 2.01x10^{-8}T^{3}$ J/kg/K
$14749 - 3.51T - 7.76x10^{-3}T^{2} - 5.08x10^{-6}T^{3} + 1.22 x10^{-9}T^{4} J/kg/K$
$1752 + 0.251T + 3.94x10^{-4}T^{2} + 1.22x10^{-7}T^{3}$ J/kg/K
$150.2 + 3.55T - 4.97x10^{-3}T^2 + 3.25x10^{-6}T^3 - 7.81x10^{-10}T^4$ J/kg/K
520.64 J/kg/K
$1009.1 + 0.0251T + 8.03x10^{-5}T^2$ J/kg/K
$-1.84x10^{-5} + 9.29x10^{-8}T + 8.240x10^{-11}T^2 m^2/s$
$-8.11x10^{-5} + 3.98x10^{-7}T + 3.12x10^{-10}T^2 m^2/s$
$-1.79 x 10^{-5} + 9.44 x 10^{-8} T + 1.31 x 10^{-10} T^2 m^2/s$
$-1.31x10^{-5} + 6.71x10^{-8}T + 6.34x10^{-11}T^2 m^2/s$
$-1.80 x 10^{-5} + 8.95 x 10^{-8} T + 7.79 x 10^{-11} T^2 m^2/s$

k <sub>0,gasif</sub>	0.467 mol/s/m <sup>2</sup> /Pa
Eagasif	186.6 kJ/mol
$k_{0,WGS,f}$	2.78 m <sup>3</sup> /mol/s
$Ea_{WGS,f}$	12.56 kJ/mol
Keq	0.02086 <i>exp</i> (4372.1/T)
η	1
$H^{\theta}_{f,CO}$	-110.525 kJ/mol
$H^{0}_{f,H2}$	0 kJ/mol
$H^{0}_{f,H2O}$	-241.818 kJ/mol
$H^{\theta}_{f,CO2}$	-393.509 kJ/mol
$H^{ heta}_{f,C}$	0 kJ/mol
$S^{0}_{CO}$	197.66 J/mol/K
$S^{0}_{H2}$	130.68 J/mol/K
$S^{0}_{H2O}$	188.84 J/mol/K
$S^{0}_{CO2}$	213.79 J/mol/K
$S^{0}_{C}$	5.6 J/mol/K

Table 5.9: Simulation input parameters: reaction parameters

## 5.7.2 Simulation results

Temperature and velocity profiles are illustrated in Figure 5.18 for both a vertical and horizontal cross-section of the receiver geometry with silicon carbide tubes and the conditions enumerated in Table 5.10.

T <sub>0</sub> , T <sub>ext</sub>	300 K
$m_{C,0}$	0.5 g/min per tube
$F_{H2O,0}$	1.865 SLPM per tube
$F_{Ar,0}$	1 SLPM per tube
$W_{C,0}$	0.1321
$W_{CO,0}$	0
<i>W</i> <sub><i>H</i>2,0</sub>	0
W <sub>H2O,0</sub>	0.3965
W <sub>CO2,0</sub>	0
$W_{Ar,0}$	0.4713
Solar	6 kW
Power	U K W
Attenuator	50%
opening	2070

Table 5.10: Simulation input parameters: operating and inlet conditions



Figure 5.18: Profiles of (a) temperature (K) and (b) vertical velocity (m/s) in vertical and horizontal receiver cross-sections

Temperature distributions are clearly non-uniform with the highest temperatures localized within a small region on the front of the center tube producing undesirably large temperature gradients both around the circumference of each tube and along the vertical dimension. These gradients are particularly large at the front of the center tube where the temperature varies by 450 K over a mere 5 cm length. The center tube attains temperatures nearly 450 K higher than the front tubes and 250 K higher than the back tubes under these conditions. External cavity walls are cooled to preserve surface reflectivity and the resulting temperature gradient between the heated tube and cooled cavity surfaces induces a recirculation pattern via natural convective flow. The heated

gases move upward along the heated tubes and downward along the cooled cavity walls as evidenced in Figure 5.18b. Though all tubes have identical inlet flow rates and compositions, the highest fluid velocities are attained in the center tube due to a comparatively larger contribution from thermal gas expansion and generation of gaseous species by reaction.

As a result of the unidirectional nature of the solar heat source, sizeable temperature gradients develop around the surface of each tube and are largest for tubes positioned closest to the focal point. Figure 5.19 displays temperature profiles around the circumference of each of three tubes at a vertical position aligned with the window centroid with angle  $\beta$  measured counterclockwise around the tube surface from the direction facing the window. Figures 5.5 and 5.8 reveal that a preponderance of the solar energy is absorbed prior to reflection by the cavity wall, thereby producing nearly complete shielding of the back of the tube array from the solar radiation source. Correspondingly, tube front and back surface temperatures differ by as much as 340 K, 130 K, and 240 K for the center, front east, and back east tubes, respectively, and the large gradients imposed over the 2.54 cm tube diameter highlight potential material concerns.



Figure 5.19: Temperature profiles around the tube circumference at a vertical position aligned with the aperture centroid

Radial profiles of temperature and velocity in the vertical (*y*) dimension are illustrated in Figure 5.20 as a function of the dimensionless vertical *y*-coordinate with y/L = 0 defined at the tube inlet.



Figure 5.20: Radial profiles within the center tube of (a) velocity in the vertical (y) dimension and (b) fluid temperature

Profiles in the top half of the tube are shown in solid lines whereas those in the bottom half of the tube are depicted by grey dashed lines. Thermal gas expansion produces a nearly five-fold increase in the centerline gas velocity between the inlet and the hot zone. Yet despite the laminar

flow pattern and high gas velocity, temperature at the tube centerline reaches values nearly equivalent to surrounding wall temperatures within the hot zone owing to radiative exchange between carbon particles and tube walls. Figure 5.21 displays the fluid temperature at the centerline of the center tube as a function of dimensionless vertical position alongside corresponding front and back surface temperatures.



Figure 5.21: Center tube wall and centerline fluid temperatures predicted with and without absorption of radiative energy

The fluid/particle mixture absorbs radiative energy emitted by the hot front wall and re-emits a portion of this energy toward the comparatively cooler back wall. As such the centerline fluid/particle temperature tracks closely with wall temperatures and attains a value intermediate to the highest and lowest temperatures of surrounding surfaces in the hot zone. Outside of the heated length, the centerline temperature drops rapidly due to radiative exchange between the heated fluid/particle mixture and the comparatively cooler tube walls. The dashed line in Figure 5.21 results from an analogous simulation in which the absorption coefficient is artificially set to zero and represents the centerline temperature predicted by purely convective and conductive heat transfer in the absence of radiative exchange. Heat transfer by convection and conduction is

ineffective compared to radiative exchange and produces a substantially reduced maximum temperature which occurs near the bottom of the tube.

Carbon, CO, and CO<sub>2</sub> mass fractions in a vertical slice of the center tube are displayed in Figure 5.22. The steam gasification reaction occurs preferentially near the front wall in regions of high temperature whereas carbon dioxide production by the water gas shift reaction is favored by equilibrium at comparatively lower temperatures which occur near the bottom of the tube.



Figure 5.22: Mass fraction of C, CO and  $CO_2$  in a vertical slice of the center tube

Thermophoresis produces net movement of particles away from heated walls in the top region of the tube, toward the relatively cooler back wall in the hot zone, and finally toward the cooled walls in the lower region of the tube. The net effects of thermophoretic diffusion are apparent in radial profiles of carbon mass fraction in the center tube illustrated in Figure 5.23. The combination of thermophoretic and convective transport produce slight local maxima in carbon mass fraction near the tube walls. Fluid velocity remains comparatively low in the region

of these maxima allowing for local spatial accumulation of carbon particles which entered the tube near the solid wall. In the center of the tube diminished thermal gradients and comparatively larger convective flow negate the effects of thermophoretic diffusion.



Figure 5.23: Radial profiles of carbon mass fraction in the center tube

Simulations excluding thermophoretic diffusion permit more carbon to remain immediately next to tube walls where both temperature and residence time are larger than the corresponding values in the tube interior. The resulting carbon conversion exceeds that shown here by approximately 4%. Combined carbon, CO, and CO<sub>2</sub> mass flow as a function of vertical position indicate that carbon deposition on tube walls only occurs within the lower cooling zone below the cavity and, for the conditions in Table 5.10, deposition removes roughly 5% of the carbon particles introduced at the tube inlet.

The cumulative residence time distribution (RTD) for the center tube is shown in Figure 5.24 along with distributions for an ideal isothermal laminar flow reactor (LFR) with either an identical minimum ( $t_{min} = 0.4$  s) or average residence time ( $\tau = 1.7$  s). The actual minimum residence time is less than half that for an ideal isothermal LFR with the same average residence

time because of gas expansion and the corresponding augmented velocity at the tube centerline. The RTD depicted in Figure 5.24 is assessed for the entire tube length including cooled regions. However, more than 80% of carbon conversion occurs within less than 15% of the tube length in a region where fluid velocity is maximized signifying that residence time in the heated length is a mere fraction of the total residence time.



Figure 5.24: Cumulative residence time distribution for the center tube

Overall carbon conversion to CO and CO<sub>2</sub> in the center tube is depicted in Figure 5.25 as a function of dimensionless vertical position. Carbon conversion is evaluated from local CO and CO<sub>2</sub> mass fractions and fluid properties via equation 5.82 where  $\rho$  is the mixture density,  $v_y$  is the *y*-velocity and the integrals are carried out numerically over the tube cross section at a specified vertical position. The denominator represents the molar flow rate of carbon at the tube inlet.

$$X = \frac{\iint \left(\frac{w_{CO}}{MW_{CO}} + \frac{w_{CO_2}}{MW_{CO_2}}\right) \rho \upsilon_y dA}{\iint \left(\frac{w_{C,0}}{MW_C}\right) \rho_0 \upsilon_{y,0} dA}$$
(5.82)



Figure 5.25: Carbon conversion and centerline fluid temperature within the center tube as a function of vertical position

Carbon conversion occurs predominantly within the length of tube situated directly in front of the receiver window. Vertical and radial profiles for the back and front tubes are entirely analogous to those shown in Figures 5.20-5.25 for the center tube, with the exception of lower overall temperatures and reaction conversion.

Table 5.11 lists the maximum surface temperature, mass-weighted average fluid temperature in the horizontal plane aligned with the aperture centroid, total reaction conversion, absorbed solar energy, and net absorbed radiative energy for the operating conditions in Table 5.10.

Tube	T <sub>max</sub> (K)	Fluid $T_{avg}(\mathbf{K})$ at $y = 0$	Q <sub>abs,solar</sub> (W)	Q <sub>abs,net</sub> (W)	Reaction conversion
Center	1813	1581	1950	832	40.4%
Front East	1343	1257	465	660	2.5%
Back East	1526	1363	981	705	9.2%

 Table 5.11: Comparison of temperature, reaction conversion and absorbed energy between tubes for a 6 kW solar power input

The center tube absorbs 33% of the total solar energy; nearly twice that absorbed by the back tube and more than four times that absorbed by the front tube. Radiation exchange between tubes results in net transfer of energy from the hotter center and back tubes to the comparatively cooler front tubes leading to more uniform temperature distributions than would be expected from the solar component alone. Temperature variability between tubes results in highly non-uniform reaction conversion with values ranging from 2.5 - 40%. Low reaction conversion severely limits receiver efficiency as net absorption by the outer tubes accounts for 45% of the solar input, but each outer tube fails to achieve temperatures high enough to carry out the gasification reaction to a significant extent.

Solar-to-chemical receiver efficiency is defined in equation 5.83 as the fraction of the incident solar power used to carry out the endothermic chemical reaction including sensible enthalpy requirements for the reactive components. Sensible enthalpy requirements for inert components or unconverted reactants are neglected.

$$\eta = \frac{\sum_{i}^{tubes} X_{C,i} \dot{n}_{Co,i} \Delta H_r(T_{avg,i}) + X_{C,i} \dot{n}_{Co,i} \int_{T_{inlet}}^{T_{avg,i}} (\hat{C}_{p,C} + C_{p,steam}) dT}{Q_{solar}}$$
(5.83)

 $X_{C,i}$  is the total carbon conversion in tube *i*, and  $\dot{n}_{Co,i}$  is the inlet molar flow rate of carbon to tube *i*.  $T_{avg,i}$  is defined as the mass averaged fluid temperature in tube *i* at the horizontal plane aligned with the aperture centroid, and is computed via equation 5.84.

$$T_{avg,i} = \frac{\iint T\rho \left| \vec{\upsilon} \cdot d\vec{A} \right|}{\iint \rho \left| \vec{\upsilon} \cdot d\vec{A} \right|}$$
(5.84)

The receiver efficiency is a mere 1.5% for the conditions listed in Table 5.10. The efficiency based purely on chemical enthalpy is 1% indicating that 33% of the energy consumption comes from sensible enthalpy requirements for reactive components. The maximum achievable

efficiency based on complete conversion of the carbon feed is only 11.2% for these conditions. While the limiting value may be increased via larger carbon feed rate, the concomitant increase in steam flow necessary to maintain at least a stoichiometric steam to carbon ratio leads to diminished residence time and conversion. Simulations carried out with an augmented carbon feed rate of 2 g/min per tube and the requisite stoichiometric steam feed rate produce a solar-to-chemical efficiency of 3.7% with a projected 44.5% efficiency at complete carbon conversion. However, overall carbon conversion is 30-40% lower than the values in Table 5.11 because of a correspondingly shorter residence time. In each case the efficiency limitation imposed by the carbon feed rate is more restrictive than the idealized absorption efficiency described in Chapter 2.

The distribution of radiative and convective/conductive heat losses is provided in Table 5.12 as a function of solar power input corresponding to attenuator openings of 10%, 25%, 35%, and 50% with assumed direct normal insolation of 1 kW/m<sup>2</sup>.

Solar power (kW)	Solar radiation Reflection Absorption		<b>Emitted ra</b> Transmission	adiation Absorption	Convection / Conduction
1.2	13.6%	6.3%	3.3%	7.5%	69.3%
3.1	12.9%	6.8%	6.0%	11.7%	62.5%
4.4	12.7%	7.3%	7.3%	14.0%	58.8%
6.1	12.3%	7.5%	8.5%	16.3%	55.4%

Table 5.12: Heat loss distributions as a function of incident solar power

Solar reflection losses include energy reflected at the exterior window surface as well as that which penetrates through the window surface, but is lost by transmission after any number of reflections within the cavity or window interior. Solar absorption losses account for solar energy absorbed by all actively cooled surfaces. The fraction of solar energy lost by either reflection or absorption is only a weak function of solar input with slight discrepancies attributable to flux profile variability with respect to attenuator opening. Energy emitted by heated structures can be lost by either transmission through the transparent window or absorption by actively cooled surfaces. Increases in emission losses with incident solar power stem from corresponding increases in tube surface temperatures. Convection and conduction losses are, for all conditions, more substantial than radiative losses and are subdivided in Table 5.13.

Solar power (kW)	cavity walls	cavity top + tube tops	cavity bottom + tube bottoms	window
1.2	0.5%	38.3%	30.7%	0.3%
3.1	2.3%	33.1%	27.0%	0.7%
4.4	2.0%	30.9%	25.7%	0.8%
6.1	1.4%	29.0%	24.7%	0.8%

Table 5.13: Convective and conductive heat losses as a function of solar power input

Convective and conductive losses occur predominantly at the top and bottom of the receiver cavity and can be primarily attributed to conduction of absorbed energy along the length of the tubes to the upper and lower cooling zones. Convective losses are marginally higher at the top of the cavity than the bottom due to the influence of natural convection within the cavity fluid. Heated fluid rises along tube surfaces and transfers energy to the top cooling zone rather than the cylindrical cavity walls. Though net convective and conductive losses decrease with solar power, the relative distribution among regions in Table 5.13 remains stable with 52-54% of convective and conductive losses resulting from the cavity top and tube tops and 43-44% resulting from cavity bottom and tube bottoms.

### 5.7.3 Evaluation of east/west symmetry assumption

The total radiative energy is broken into two components: shorter-wavelength solar energy introduced through the aperture, and longer-wavelength (IR) energy emitted by heated surfaces. The solar component is treated via the Monte Carlo model within the entirety of the receiver whereas the emitted component is treated with a coupled finite volume and CFD model, both of which are solved exclusively in the hotter east half of the receiver with assumed east/west symmetry. In actuality temperatures on the west side fail to match those on the east due to a slightly asymmetric solar flux profile and the coupled finite volume/CFD simulation is repeated for the cooler west side to quantify error incurred by the symmetry assumption. Resultant maximum temperatures obtained from the west side simulation are 1741 K, 1273 K, and 1460 K for the center, front west, and back west tubes respectively compared to corresponding values of 1813 K, 1343 K, and 1526 K obtained for the east side. Table 5.14 presents the solar and emitted (IR) energy absorbed by each surface alongside the average absorbed IR energy between individual east and west simulations for the operating conditions in Table 5.10.

	Qabs, solar, east (kW)	Qabs, solar, west (kW)	Qabs, IR, east (kW)	Q <sub>abs, IR, west</sub> (kW)	Qabs, IR, average (kW)
Center tube	1.95	1.89	1.74	1.52	1.63
Front tube	0.47	0.40	1.52	1.33	1.43
Back tube	0.98	0.90	1.51	1.33	1.42

Table 5.14: Solar and emitted (IR) energy absorbed in individual east and west side simulations

Realistically the longer-wavelength IR energy absorbed in the east half of the receiver originates from emission on both east and west sides implying that the actual quantity absorbed on the east side lies somewhere between the extremes in Table 5.14. Given the proximity and

correspondingly larger view factors between tubes on the same side of the receiver than between those on opposing sides, the actual quantity of IR energy absorbed on the east side should be more heavily weighted by the value from the east simulation than that from the west. Thus a worst-case scenario estimate of the error present in the total absorbed energy can be generated using an unweighted average of absorbed IR energy from the two individual simulations. This unweighted average is approximately 6% lower than the absorbed IR energy calculated from the east side simulation alone and absorbed IR energy represents only 47%, 77%, and 61% of the total absorbed energy for the center, front, and back tubes respectively. Therefore the maximum 6% error in absorbed IR energy translates into at most 3-5% error in the total absorbed energy, or less than 0.1 kW per tube.

#### 5.7.4 Angular and spatial mesh verification

Computational fluid dynamics model solutions are obtained on various angular and spatial grids in order to ensure an adequate number of mesh elements and to verify solution independence from mesh element size and angular discretization. Grid independence is evaluated individually for the regions interior and exterior to the absorber tubes. To assess grid independence in the cavity space, solutions are obtained with a total number of spatial mesh elements equal to 191,958, 295,864, 385,632, and 555,642. These spatial grids have, respectively, 87,780, 130,410, 226,710, and 366,900 elements in the cavity fluid. Angular discretization is described by ( $N_{\theta} \times N_{\phi}$ ) = (5x5), (7x7), (9x9), and (11x11) with  $8N_{\theta} N_{\phi}$  equations associated with the finite volume radiation model solved within each spatial mesh element. All spatial grids are generated with a comparatively higher element density in a boundary layer surrounding each solid surface. Profiles of temperature and incident emitted (IR) radiative energy flux are compared around the circumference of each tube for eight vertical positions

spanning the tube length. All simulations are carried out with purely inert gas flow and a solar input of 8.5 kW. This corresponds to an attenuator opening of 100% and is selected such that mesh independence is evaluated under conditions of maximum temperature and emitted radiative energy. Table 5.15 provides the maximum error at any point along each tube surface calculated relative to solutions on a spatial grid with 555,642 elements and  $(N_{\theta} x N_{\Phi}) = (9x9)$ . Table 5.16 identifies the maximum error relative to an angular grid described by  $(N_{\theta} x N_{\Phi}) = (11x11)$  with a spatial grid of 295,864 mesh elements.

Mesh elements	Temperature	Incident radiation (excluding solar)
191,958	35 K (3%)	36 kW/m <sup>2</sup> (22%)
295,864	28 K (2%)	34 kW/m <sup>2</sup> (20%)
385,632	7 K (1%)	12 kW/m <sup>2</sup> (5%)

Table 5.15: Maximum errors relative to solutions on a spatial grid of 555,642 elements with  $(N_{\theta} x N_{\phi}) = (9x9)$ 

Table 5.16: Maximum errors relative to solutions on an angular grid of  $(N_{\theta} x N_{\phi}) = (11x11)$  with 295,864 spatial mesh elements

$\begin{array}{c} N_{\theta} = \\ N_{\Phi} \end{array}$	Temperature	Incident radiation (excluding solar)
5	4.3 K (0.4%)	7.3 kW/m <sup>2</sup> (9%)
7	2.7 K (0.2%)	3.0 kW/m <sup>2</sup> (3%)
9	1.6 K (0.1%)	$1.1 \text{ kW/m}^2 (2\%)$

Maximum error and maximum fractional error may occur at distinct locations, but both frequently arise at the back of the center tube in the horizontal plane aligned with the aperture centroid. The solution is more sensitive to the spatial than the angular grid at these element sizes and, based on the results in Tables 5.15 and 5.16, an optimal mesh of 385,632 elements with  $(N_{\theta} x N_{\phi}) = (7x7)$  is selected. Maximum error in incident emitted (IR) radiative flux may be as high as 5% yet, as the IR energy represents only a fraction of the total absorbed energy, tube surface temperature errors are under 10 K or less than 1% of the predicted temperature. These results reveal that additional refinements in the spatial or angular grids, and the associated increase in computational requirements, are unnecessary.

Interior tube spatial grids are evaluated for reacting flows under realistic conditions. Operating conditions are modified to 2 SLPM argon and 0.5 g/min carbon per tube, with 4.2 kW solar power and an initial molar steam to carbon ratio of 1.5. Two initial spatial grids are generated independently with 17,934 and 108,486 mesh elements contained within half of the center tube and are characterized by comparatively higher element density in a boundary layer surrounding tube walls. The mesh comprised of 17,934 elements is then refined in regions characterized by rapid gasification reaction rate or large gradients in carbon mass fraction in order to generate additional spatial grids consisting of 35,224 and 35,280 elements respectively. Solution profiles are evaluated within the tube fluid along the vertical coordinate at each of five locations evenly spaced between the front and back of the tube.

Table 5.17 lists the maximum error in the hot zone temperature, velocity in the vertical direction, density, overall carbon conversion, and mass fraction of C, CO, H<sub>2</sub>, and CO<sub>2</sub> relative to the solution on a spatial grid with 108,486 elements with ( $N_{\theta} x N_{\phi}$ ) = (5x5). These errors are also recast as the percentage of the maximum value attained in the tube. Solutions obtained on the spatial mesh of 17,934 elements exhibit considerable error near the front of the tube in the hot zone where gasification occurs rapidly. Thus, not surprisingly, the spatial grid created through addition of elements in regions of rapid gasification rate produces the best solution compared to the spatial grid of 108,486 elements. Component species mass fraction errors with this spatial grid are at most 2% and typically fall below 1%.

	Mesh elements		
	17,934	35,280	35,224
<i>T</i> (K)	15 (1%)	13 (1%)	12 (1%)
$v_y$ (m/s)	0.04 (2%)	0.04 (2%)	0.04 (2%)
$\rho (\text{kg/m}^3)$	0.05 (3%)	0.05 (3%)	0.05 (3%)
$w_C$	0.006 (5%)	0.004 (4%)	0.002 (2%)
w <sub>CO</sub>	0.003 (4%)	0.002 (2.4%)	7x10 <sup>-4</sup> (0.8%)
$W_{H2}$	2x10 <sup>-4</sup> (3%)	1x10 <sup>-4</sup> (1.4%)	$2x10^{-5}$ (0.3%)
W <sub>CO2</sub>	0.001 (2%)	5x10 <sup>-4</sup> (1.1%)	4x10 <sup>-4</sup> (0.9%)
Total conversion	0.011 (3%)	0.006 (2%)	0.002 (0.5%)

Table 5.17: Maximum errors relative to solutions on a center tube spatial grid of 108,486 mesh elements with  $(N_{\theta} x N_{\phi}) = (5x5)$ 

Table 5.18 provides errors in temperature and total conversion along with carbon, CO, and H<sub>2</sub> mass fractions for a simulation with  $(N_{\theta} \times N_{\phi}) = (5x5)$  relative to  $(N_{\theta} \times N_{\phi}) = (9x9)$  on a spatial grid with 17,934 mesh elements in half of the center tube. Decreasing the number of solid angles in the finite volume model produces errors well under 1% of the maximal values indicating that solutions are considerably more sensitive to the spatial than the angular grid. Results in Tables 5.16 and 5.18 imply that an angular grid defined by  $(N_{\theta} \times N_{\phi}) = (7x7)$  is sufficient for both the non-participating medium in the cavity space and the strongly absorbing, emitting, scattering medium present in the tubes.

	Error
<i>T</i> (K)	0.5 (0.03%)
$w_C$	1x10 <sup>-4</sup> (0.09%)
W <sub>CO</sub>	8x10 <sup>-5</sup> (0.1%)
$W_{H2}$	7x10 <sup>-6</sup> (0.1%)
Total conversion	4x10 <sup>-4</sup> (0.1%)

Table 5.18: Maximum errors in a simulation with  $(N_{\theta} x N_{\phi}) = (5x5)$  relative to  $(N_{\theta} x N_{\phi}) = (9x9)$  with a center tube spatial grid of 17,934 elements

### 5.7.5 Comparison with perfectly mixed ideal plug flow solution

Flow through the tubes in the three-dimensional steady state computational fluid dynamics model is characterized by laminar flow patterns and imperfect mixing. For comparison, a simplified perfectly mixed plug flow solution is evaluated with an average heat flux at the tube wall identical to that determined from the CFD model. Neglecting radial and azimuthal variations, axial dispersion, thermophoretic diffusion, and the normal component of the viscous stress tensor ( $\tau_{yy}$ ) the continuity, momentum, and species equations can be simplified to equations 5.85 – 5.87 where  $\xi_i$  is the stoichiometric coefficient for reactant species *i*.

$$\frac{d}{dy}(\rho v_y) = 0 \tag{5.85}$$

$$\rho \upsilon_{y} \frac{d\upsilon_{y}}{dy} = -\frac{dp}{dy} + \rho g_{y}$$
(5.86)

$$\rho \upsilon_{y} \frac{dw_{i}}{dy} = \xi_{i} M_{i} R_{rxn}$$
(5.87)

The volumetric molar reaction rate is given by equation 5.88 where  $k_s$  is the intrinsic surface reaction rate constant and the quantity in brackets represents the mole fraction of steam in the gas mixture.

$$R_{rxn} = \eta k_s \hat{A}_s \rho w_c p \left[ \frac{w_{H2O} / M W_{H2O}}{\sum_{gas} w_i / M W_i} \right]$$
(5.88)

Profiles of the energy flux at the interior tube wall as a function of position are extracted from the CFD simulations and averaged over horizontal planes to yield an average heat flux as a function of vertical position. These profiles are inserted into the plug flow energy equation as a volumetric source function so as to eliminate the necessity of direct solution for the divergence of the radiative flux vector. This assumption implies that the energy flux leaving the interior tube wall at a given vertical position is absorbed directly into the fluid within the same horizontal plane. In reality, the hemispherical distribution of energy emitted at a given plane will be absorbed into the fluid in locations both above and below the plane containing the emitting element. Thus while the total quantity of energy transferred into a given tube is forced to match the corresponding value obtained from the CFD model, the distribution of this energy is vastly simplified. Neglecting radial variations, axial conduction, kinetic energy terms, and viscous dissipation the energy equation is written in equation 5.89 where  $q_f''(y)$  is the average energy flux entering the tube at a given vertical position.

$$\rho \upsilon_{y} \sum w_{i} C p_{i} \frac{dT}{dy} = \frac{2q_{f}^{"}(y)}{R_{i}} - R_{rxn} \Delta H(T)$$
(5.89)

To close the system of ordinary differential equations the volume weighted average mixture density in equation 5.37 is recast in equation 5.90.

$$\rho \approx \frac{\rho_g}{1 - w_c} = \frac{p}{RT \sum_{gas} w_i / MW_i}$$
(5.90)

The resulting initial value problem is solved numerically via a simple Euler method with step size equal to 0.15% of the tube length and specified inlet temperature, mass fractions, and total mass flux. Figure 5.26 displays the plug flow temperature as a function of scaled vertical position alongside the centerline fluid and front or back interior wall temperature from the CFD simulation. The plug flow solution contains a sharp peak temperature, likely a direct result of the assumption that the energy flux leaving the interior tube wall at a given horizontal plane is absorbed directly into the fluid within the same plane. Fluid temperatures at y/L = 0.5 are 1586 K, 1229 K, and 1344 K with corresponding carbon conversion of 60%, 4.7% and 16% for the center, front east, and back east tubes respectively, comparable to the values from the CFD

simulation in Table 5.11. Comparatively higher carbon conversion results from slightly higher maximum temperature and longer residence time compared to that assessed for the laminar flow pattern. However, these results signify that the conversion can only be marginally improved with perfect mixing, particularly in the outer tubes, and thus radial temperature variations within the tube fluid are not solely to blame for low conversion. This behavior is not unexpected as the presence of strongly absorbing carbon particles results in substantially greater uniformity in interior fluid temperature than would be expected from convective and conductive heat transfer alone.



Figure 5.26: Center tube temperature profiles obtained via a three-dimensional CFD model and a simplified plug flow solution

## 5.7.6 Comparison with water-gas shift equilibrium compositions

The contributions of both forward and reverse water-gas shift reactions are frequently included in fixed, moving, or fluidized bed gasifier models above 1000°C through the assumption of water-gas shift equilibrium at local fluid conditions [71-73]. However, the short residence time considered in this study has the potential to invalidate this assumption. Figure 5.27 illustrates the mole fraction of carbon monoxide in the gas phase at the centerline of the

center tube as a function of scaled vertical position calculated from the CFD model described above using the water gas shift kinetic parameters from Biba et al.[66]. Operating conditions are modified from those in Table 5.10 to 2 SLPM argon and 0.5 g/min carbon per tube, with 4.2 kW solar power and an initial molar steam to carbon ratio of 1.5. Figure 5.27 also depicts the corresponding CO mole fraction predicted via the assumption of water-gas shift equilibrium as well as that predicted with a kinetic rate 100 times faster than the actual rate. The equilibrium assumption is clearly violated for this system as the residence time is too short to permit approach to the equilibrium composition.



Figure 5.27: Comparison of CO mole fraction predicted with either water gas shift reaction kinetic rates or equilibrium assumption

# 5.8 Sensitivity Analysis

Variability in model results arising from uncertainty in input parameters and material properties is assessed in Table 5.19 for simulations with 1.2 g/min carbon per tube, stoichiometric steam, and a total solar power input of 7 kW. Maximum temperature and carbon conversion (X) within the center and front east tubes are evaluated along with overall receiver

efficiency ( $\eta$ ). Alteration of individual input parameters by ±15% produces at most a 60 K increase in temperature, a 0.06 increase in the fractional carbon conversion, and a 0.015 increase in the fractional receiver efficiency. Thus while the simulation cannot be deemed entirely insensitive to input parameters, reasonable modifications of these parameters fail to substantially improve predicted receiver performance.

Base r	esults	T <sub>max,,center</sub> 1874 K	<i>T<sub>max,,FE</sub></i> 1413 К	$X_{center}$ 0.404	$X_{FE}$ 0.047	$\eta$ 0.036
		Change (% Change)				
Property	Change	T <sub>max,,center</sub>	$T_{max,,FE}$	Xcenter	$X_{FE}$	η
$k_{SiC}$	+ 15%	-22 (1%)	-27 (2%)	-0.022 (6%)	-0.011 (24%)	-0.0039 (17%)
$ ho_{cav}$	+ 15%	20 (1%)	58 (4%)	0.055 (14%)	0.051 (108%)	0.014 (58%)
$lpha_{SiC}$ , $arepsilon_{SiC}$	- 15%	-26 (1%)	-16 (1%)	-0.017 (4%)	-0.0054 (11%)	-0.0029 (12%)
$Q_{abs}$	+ 15%	1 (0.08%)	1 (0.08%)	0.005 (1%)	0.001 (2%)	0.0006 (2%)
$Q_{sca}$	+ 15%	-0.03 (<0.01%)	0.001 (<0.01%)	-6x10 <sup>-5</sup> (0.02%)	-1x10 <sup>-5</sup> (0.03%)	-2x10 <sup>-6</sup> (<0.01%)
$\mu_{gas}$	+ 15%	0.16 (0.01%)	0.19 (0.01%)	-0.002 (0.5%)	-0.0006 (1%)	-0.0003 (1%)
$k_{gas}$	+ 15%	0.02 (<0.01%)	0.23 (0.02%)	0.0013 (0.3%)	0.0004 (0.9%)	0.0002 (0.8%)

Table 5.19: Sensitivity of simulation results to 15% variability in physical and optical properties

Model results are markedly more sensitive to variability in physical and optical properties related to solid materials, particularly cavity wall reflectivity and tube thermal conductivity, than to variability in fluid properties. An increase in cavity wall reflectivity diminishes losses attributed to absorption of both solar and emitted energy thereby enhancing the net energy absorbed by the tubes. Front tube solutions are impacted comparatively more than center tube solutions because these tubes rely more heavily on cavity wall reflections to deliver the incident energy. A 15% increase in cavity wall reflectivity raises the front tube temperature by nearly 60 K and more than doubles carbon conversion attained in the front tube, yet only increases fractional receiver efficiency by 0.014 because conversion in the outer tubes remains low. Sensitivity of model results to tube thermal conductivity is not surprising given that nearly 50% of the incident solar energy is lost within top and bottom cooling zones and largely attributed to conduction along the length of the tubes. Increasing the tube thermal conductivity by 15% decreases the maximum tube temperatures by 20-30 K as energy is more readily transported away from the hot spot located in front of the aperture. The resultant decrease in fractional carbon conversion is at most 0.01-0.02 per tube leading to minimal change in receiver efficiency.

Variability in tube emissivity affects both absorption and emission and the competing effects combine to reduce the sensitivity of model results to surface emissivity or absorptivity. The absorption effect appears to dominate with a 16-26 K decrease in maximum tube temperature arising from a 15% decrease in surface emissivity. Results are slightly more sensitive to absorption than scattering efficiency because, as shown in Figure 5.11, the extinction coefficient for 42 nm acetylene black particles is unmistakably dominated by absorption. However, this observation is expected to hold true even in strongly scattering media since the absorption coefficient controls the net quantity of energy absorbed by the medium via the divergence of the radiative flux vector, whereas the scattering coefficient impacts only the relative distribution of intensity within the medium. Simulation results are unexpectedly insensitive to the absorption efficiency, likely on account of a limited range of variability.

Results are also insensitive to variations in gas viscosity and thermal conductivity as heating of the fluid/particle mixture is accomplished predominantly by radiative exchange.

Variations in particle diameter, density, and specific surface area as the reaction progresses may be described via a number of existing reaction models. The shrinking particle model assumes all reaction occurs on the external particle surface producing no change in particle density, whereas the progressive conversion model assumes reaction occurs throughout the interior of a porous particle potentially leading to a decreasing particle density with constant particle size. Modifications in specific surface area with reaction conversion can be complex [51] and, for lack of detailed information, the particles in this study are assumed to retain a constant specific surface area. Table 5.20 shows the variability in CFD model results predicted for 15-100% changes in particle diameter, density, and specific surface area with operating conditions identical to those used to generate Table 5.19.

		<u>Change (% Change)</u>				
<u>Property</u>	<u>Change</u>	T <sub>max,, center</sub> (K)	T <sub>max,,FE</sub> (K)	Xcenter	$X_{FE}$	η
$d_p$	- 50%	8.2 (0.4%)	5.2 (0.4%)	0.020 (5%)	0.0040 (8%)	0.0022 (6%)
$ ho_C$	- 50%	8.2 (0.4%)	5.3 (0.4%)	0.019 (5%)	0.0038 (8%)	0.0021 (6%)
$\hat{A}_s$	+ 15%	-1.2 (0.07%)	-0.9 (0.06%)	0.021 (5%)	0.0054 (12%)	0.0026 (7%)
$\hat{A}_s$	+ 50%	-3.8 (0.2%)	-3.2 (0.2%)	0.060 (15%)	0.017 (35%)	0.0075 (21%)
$\hat{A}_s$	+ 100%	-3.9 (0.2%)	-1.4 (0.1%)	0.16 (41%)	0.036 (77%)	0.018 (51%)

Table 5.20: Sensitivity of simulation results to 15-100% variability in particle properties

As discussed in section 5.5.4, provided the assumptions behind the single fluid mixture model are not violated, particle diameter only directly impacts particle diffusivity and absorption or scattering coefficients. In the Rayleigh limit, the absorption coefficient and scattering phase function become independent of particle size whereas the scattering coefficient is proportional to the third power of particle diameter. However, Table 5.19 indicates that simulation results are altogether insensitive to scattering efficiency, so the 87% drop in scattering projected by a 50% decrease in particle size should yield minimal impact on solutions from the CFD model. Conversely, a 50% drop in particle diameter produces a nearly four-fold increase in Brownian diffusion which partially counteracts the effects of themophoretic diffusion producing comparatively higher particle concentrations in heated regions and thereby leading to slightly higher carbon conversion. Maximal changes in particle size arise when reaction occurs exclusively at the external surface, yet even at this extreme more than 87% conversion of the particle material is required to reduce the particle diameter by a factor of two. Maximal changes in particle density, on the other hand, arise when reaction takes place entirely within the interior of the particle. A decrease in particle density leads to diminished fluid/particle mixture density and a correspondingly reduced fluid flow rate with longer residence time. Yet a 50% drop in particle density over the entirety of the reaction tube increases fractional reaction conversion and receiver efficiency by at most 0.02 and 0.003 respectively. The relative insensitivity of simulation results to both particle diameter and density suggest that the choice of particle reaction model is not critical for the conditions of interest.

Though local reaction rate is directly proportional to available surface area, a 50% increase in specific surface area within the entire reaction tube enhances fractional conversion by at most 0.06, 0.04, and 0.02 for the center, back, and front tubes respectively leading to a

fractional receiver efficiency higher than the base case by less than 0.01. Receiver efficiency predicted with double the specific surface area is only marginally higher. If the gasification reaction occurs exclusively at the external particle surface, the specific surface area increases weakly over the first 50-60% of particle conversion, with more than 87% conversion required to double the specific surface area. Realistically, the reaction occurs at both internal and external particle surfaces leading to a complex and unknown relationship between reaction conversion and specific surface area. However, the results in Table 5.20 suggest that the predicted receiver efficiency is not adversely impacted by the assumption of constant specific surface area, though this analysis may break down at high carbon conversion.

## 5.9 Experimental Validation

## 5.9.1 Experimental setup

On-sun experimental testing of the existing receiver is conducted at the High Flux Solar Furnace (HFSF) at the National Renewable Energy Laboratory (NREL). The HFSF is described by Lewandowski et al. [25] and consists of a single flat heliostat, a primary concentrator comprised of an array of mirrored hexagonal facets each with an identical radius of curvature, and a vertically-opposing two plate attenuator utilized to control the total power incident on the receiver with a maximum achievable solar input of roughly 9 kW. The secondary concentrator described by Dahl et al. [26] is placed in front of the receiver aperture. This concentrator narrows from an octagonal inlet to a rectangular outlet with dimensions matching those of the aperture and is capable of producing more than 3000 kW/m<sup>2</sup> peak flux with a fully open attenuator. A blackbody calorimeter is employed to correlate the power entering the secondary concentrator with the measured direct normal solar insolation and attenuator opening, thereby

allowing experiments to be carried out on the basis of consistent power input despite variations in daily atmospheric conditions.

Five distinct cooling chambers encircle the receiver at the top, bottom, front, back and window. During on-sun experimental testing the cooling chambers are connected to a closed-loop chiller flowing a 1:1 water and propylene glycol mixture. Cooling fluid flow rates are measured at the inlet of each cooling zone. Gas flow rates are adjusted via three mass flow controllers attached individually to the center tube, surrounding outer tubes, and cavity chamber. Downstream gas flow rates exiting the receiver are measured with a mass flow meter (Flow Technologies FTO series) and all gas flow devices are calibrated with a gas flow sensor (Bios International DryCal DC-2). Pressure relief valves are attached to each gas flow line in order to prevent overpressurization from thermal expansion.

Cooling fluid temperatures are measured at the inlet and exit of each of five cooling zones via type K thermocouples. Cavity wall temperature is monitored by means of eight additional type K thermocouples positioned within 1.6 mm of the reflective surface [5]. Tube temperatures are quantified with type B or type K thermocouples inserted from the top of the tube and bent to touch the internal wall within the region of the hottest point. External center tube surface temperatures are also assessed at the back of the tube in the horizontal plane aligned with the aperture centroid, and at the front of the tube in the horizontal plane aligned with the bottom of the aperture via type K thermocouples inserted through sealed ports in the outer cavity wall. A solar-blind pyrometer (Heitronics KT-19.01) is aimed through an optical port in the back cavity wall to provide an independent measurement of temperature at the back center tube wall. Pyrometer ports are sealed with quartz rods to maintain a purged cavity environment. Tubes are constructed from either silicon carbide (Hexoloy SA SiC) or Inconel 600.

A brush feeder is utilized to entrain particles in a stream of argon gas and the gas/particle mixture is introduced to the center tube via a 0.32 cm outer-diameter feed tube ending below the top cooling chamber in order to minimize particle deposition in the cooled top region of the tube. Solid feed rates are restricted to 0.3-0.4 mg/s in order to prevent particle clogging in the feed lines. Water is delivered to the center tube via a syringe pump connected to a 0.16 cm outer-diameter stainless steel tube ending 5 cm below the top cooling chamber. The fluid/particle mixture from the center tube flows through a gravity collection vessel and is combined with the inert effluent from the outer tubes downstream from the receiver. The mixture travels through a HEPA filter and water cold trap prior to reaching a non-dispersive infrared analyzer (California Analytical Instruments Model 600) in which the CO and CO<sub>2</sub> composition of the product stream is evaluated. A typical gasification experiment was initiated by heating the receiver to the desired level with purely inert materials. Water flow to the center tube was commenced after steady state temperatures were attained with inert materials, and sustained for at least 5 min until effluent compositions equilibrated prior to the introduction of reactant particles.

### 5.9.2 Experimental validation of total solar power input

Experimental validation is accomplished in three distinct stages. First the total power at the secondary concentrator exit is measured with a blackbody calorimeter in place of the solar receiver and compared to the total solar power predicted by the SolTrace model as a function of attenuator opening. Second, temperature profiles are assessed under inert flow conditions and compared with results from the combined Monte Carlo, finite volume, and CFD model. Finally, the extent of carbon gasification is quantified experimentally as a function of solar power input and compared with corresponding values from the theoretical model using kinetic parameters available in the literature. Figure 5.28 displays experimentally measured values of total power

at the secondary concentrator exit plane adjusted to a specified direct normal solar insolation of  $1000 \text{ W/m}^2$ . Actual direct normal insolation varied between  $1014-1025 \text{ W/m}^2$  during experimentation and the resultant solar power measurements are scaled linearly to adjust to the specified insolation. Experimental data are compared to predictions from the SolTrace model detailed in section 5.3.1 for various values of the unknown secondary concentrator reflectivity. Alteration of the reflectivity adjusts the vertical position of the curve arising from the SolTrace model with negligible change in shape. Superior quantitative predictions occur with a reasonable 73% secondary concentrator reflectivity.



Figure 5.28: Experimentally measured and theoretically predicted solar power at the secondary concentrator exit

All experimentally measured receiver temperature profiles are compared with theoretical predictions on the basis of the experimentally measured solar power incident on the receiver window. Thus the estimated secondary concentrator reflectivity impacts the theoretically predicted temperature only through the shape and directionality of the solar flux profile by means of the attenuator opening necessary to achieve the given solar power input. A 73% secondary concentrator reflectivity necessitates an attenuator opening only 3% higher than that predicted with a 95% reflectivity for any power input below 7 kW. Results in section 5.3 suggest that

variability in the shape and directionality of the flux profile may be neglected over this narrow range thereby rendering the theoretically predicted temperature profiles essentially insensitive to the secondary concentrator reflectivity.

### 5.9.3 Experimental validation for temperature profiles

Temperature profiles are evaluated for both a metallic (Inconel 600) and ceramic (silicon carbide) tube material under inert conditions with argon flow rates maintained at 1 SLPM in the center tube and 0.5 SLPM in each of the four surrounding tubes. The nominal solar power input is defined from existing correlations relating the solar power entering the secondary concentrator to the direct normal solar insolation and attenuator opening. Attenuator opening is adjusted automatically during experimentation in response to temporal variations in direct normal insolation in order to maintain a constant nominal power input. Experiments with silicon carbide tubes installed in the receiver are conducted over a nominal solar power range of 1.5 - 7 kW whereas nominal power is restricted to 3 kW for experiments with Inconel tubes so as to maintain tube temperatures below  $1150^{\circ}$ C and preclude localized tube melting. The solar power incident on the external window surface cannot be measured directly during on-sun tests and is inevitably lower than the nominal power input as a fraction of the energy is lost by absorption at the secondary concentrator surface or transmission through a small gap separating the secondary concentrator exit plane from the receiver window.

Two independent estimates of the solar power incident on the receiver window ( $Q_{wind}$ ) are generated by equations 5.91 and 5.92 using parameters identified in Figure 5.29.

$$Q_{wind,1} = Q_{conc} - Q_{gap} = Q_{conc} (1 - f_{gap})$$
(5.91)

$$Q_{wind,2} = Q_{cond} + Q_{re-rad} + Q_{s,refl,wind} + Q_{s,refl,cav} = \frac{Q_{cond} + Q_{re-rad}}{1 - f_{s,refl,wind} - f_{s,refl,cav}}$$
(5.92)



Figure 5.29: Specification of solar energy inputs and losses

Solar power at the exit of the secondary concentrator ( $Q_{conc}$ ) is estimated from the average attenuator opening during experimentation by means of the correlation shown in Figure 5.28 for a direct normal solar insolation of 1000 W/m<sup>2</sup> and scaled linearly to adjust to the actual average direct normal insolation during experimentation. All experimental tests are carried out under conditions characterized by 880 - 1050 W/m<sup>2</sup> direct normal solar incidence. The energy lost in the gap between the secondary concentrator and receiver window ( $Q_{gap}$ ) is estimated as a fraction ( $f_{gap}$ ) of the energy exiting the secondary concentrator ( $Q_{conc}$ ) and as a function of attenuator opening. The value of  $f_{gap}$  is approximated by linear interpolation between SolTrace model calculations carried out at seven levels of attenuator opening from 10-100% and varies between 0.071 and 0.078.

A second estimate of energy incident on the receiver window surface  $(Q_{wind,2})$  is obtained from the sum of energy lost to the cooling zones  $(Q_{cond})$ , energy lost by emission through the window  $(Q_{re-rad})$ , solar energy lost by reflection at the external window surface  $(Q_{s,refl,wind})$  and solar energy which penetrates through the external window surface but is lost by transmission after some number of reflections in the interior  $(Q_{s,refl,cav})$ . Solar reflection losses are derived as fractions  $(f_{s,refl,wind}, f_{s,refl,cav})$  of the total energy incident on the window and are estimated from linear interpolation between Monte Carlo model calculations at seven values of attenuator opening between 10% and 100%. Reflection by the window surface  $(f_{s,refl,win})$  and by receiver surfaces ( $f_{s,refl,cav}$ ) accounts for 4.6-4.8% and 7.7-9.4% of the total energy incident on the receiver window ( $Q_{wind}$ ) respectively.

Energy losses in the cooling zones are computed from equation 5.93 in which  $m_i$  is the measured mass flow rate of fluid in cooling zone *i*,  $T_{in,i}$  and  $T_{out,i}$  are, respectively, the measured inlet and outlet temperatures for cooling zone *i*,  $C_p$  is the heat capacity of the cooling fluid and the summation is carried out over the five distinct cooling zones.

$$Q_{cond} = \sum_{i=1}^{5} m_i \int_{Tin,i}^{Tout,i} C_p dT$$
(5.93)

Energy lost by emission through the transparent window is estimated from the measured tube temperatures and approximate configuration factors between the tubes and window via equation 5.94.

$$Q_{re-rad} = \varepsilon_{tube} \sigma A_{tube} \sum_{i=1}^{N_{tubes}} \left[ F_{f-w,i} \left( \overline{T}_{f,i}^{4} - 300^{4} \right) + F_{b-w,i} \left( \overline{T}_{b,i}^{4} - 300^{4} \right) \right]$$
(5.94)

Configuration factors are approximated as those between the internal window surface and a constant-temperature section of tube with height identical to that of the aperture. Losses originating from emission either above or below the aperture are disregarded. Configuration factors are estimated from Monte Carlo calculations including the effects of the specularly reflective cavity wall as described in Chapter 3. These approximate configuration factors are computed separately for the front ( $F_{f-w}$ ) and back ( $F_{b-w}$ ) halves of the tube and are shown in Table 5.21.

 Table 5.21: Approximate tube - window radiation configuration factors

 predicted from Monte Carlo calculations

	$F_{f-w}$	$\overline{F}_{b-w}$
Center tube	0.128	0.0014
Front tube	0.103	0.0011
Back tube	0.050	0.012

The "front" half is designated relative to the point on the tube surface at which the distance to the window centroid is minimized. The constant average temperature for the front section of tube  $i(\overline{T}_{f,i})$  is taken to be the experimentally measured maximum temperature while that for the back section  $(\overline{T}_{b,i})$  is defined as the extrapolated temperature at a point midway between the front and back of the tube. The front/back temperature discrepancy is determined experimentally for the center tube and extrapolated from results produced by the combined Monte Carlo, finite volume, and CFD model for the outer tubes. Both front and back tube sections are characterized by a constant temperature equivalent to the maximum temperature occurring within that section and thus emission losses are slightly overestimated. However, overestimation of emission losses arising from the tube height in front of the aperture partially offsets the error introduced by excluding upper and lower tube sections. Emission losses determined from equation 5.94 account for 3-10% of the solar energy incident on the window surface.

Center tube temperature is measured at both the front and back walls in a horizontal plane aligned with the aperture centroid, and at the front wall in a horizontal plane aligned with the bottom of the aperture. Figure 5.30(a) displays center tube temperatures both measured experimentally and predicted by the theoretical model as a function of solar power incident on the external window surface. Figure 5.30(b) provides experimental measurements and theoretical predictions for temperature at the approximate maximum value attained inside the center, front east, and back east tubes. The experimental points in Figure 5.30 correspond to nominal solar power inputs of 1.5, 2, 3, 4, 5, 6 and 7 kW. Curves from the theoretical model are generated with the input parameters defined in Tables 5.5 - 5.9 which are either taken from literature and material manufacturers or calculated directly from theory.



Figure 5.30: Experimentally measured temperature profiles for SiC tubes compared with the theoretical model for (a) center tube (b) center and outer tubes

The high and low power levels designated by horizontal error bars in Figure 5.30 correspond to the two independent calculations of  $Q_{wind}$  from equations 5.91 and 5.92. Error estimates for the experimentally measured temperature are taken from the standard deviation of replicate measurements at nominal power inputs of 2, 3, 4, and 5 kW. Error estimates for temperature measured at nominal power inputs of 1.5, 6, and 7 kW are extrapolated assuming a fractional error identical to that of the closest replicated point.
The theoretical model produces both qualitatively and quantitatively accurate predictions of tube temperature at all positions except for the bottom of the window. Comparison between theoretical and experimental values at this point is hindered by large vertical temperature gradients combined with uncertainty in thermocouple position. The dashed line in Figure 5.30(a) provides the temperature predicted by the theoretical model at a point 0.5 cm above the nominal thermocouple position. Excluding the location at the bottom of the window, the average discrepancy between the theoretical prediction and experimental measurement is 44 K with the largest disparities produced at the front east tube. This average discrepancy corresponds to 4% of the measured temperature and is similar in magnitude to the experimental error. Emission losses calculated from measured tube temperatures via equation 5.94 account for 3-10% of the solar energy and increase monotonically with incident solar power. These values agree well with the theoretically predicted range of 3.3-8.5% listed in Table 5.12. Heat removed in the cooling zones accounts for 77-83% of the solar energy. This range matches closely with the 79-83% loss by convection/conduction and absorption predicted from the theoretical model in Table 5.12.

All temperature measurements are contingent on physical contact between the tube wall and the tip of the thermocouple. This cannot be verified during experimentation and may lead to systemic temperature measurement error greater than the random error identified in Figure 5.30 based on replication of individual experimental measurements. Appendix E provides approximate calculations of the discrepancy between the thermocouple and tube wall temperatures on the basis of a simple macroscopic energy balance including conduction along the length of the thermocouple to the cooled base, convective heat transfer with the surrounding fluid phase, and radiative exchange with the heated tube wall. The predicted discrepancy between thermocouple and tube wall temperatures typically exceeds the random error, particularly at low temperature when radiative exchange fails to compensate for a lack of physical contact between the thermocouple and the tube wall. Figures E.4 and E.5 illustrate the modified temperature measurement error predictions for the data in Figure 5.30(b). Comparison of Figure E.4 and Figure 5.30(b) reveals that the systemic error illustrated in Figure E.4 is only notably greater than the random error in Figure 5.30(b) at low temperature.

Figure 5.31 presents experimentally measured temperatures within each of the four outlying tubes and illustrates the typical east/west temperature disparity observed during on-sun testing. Estimated experimental errors are analogous to those in Figure 5.30 and are omitted for clarity.



Figure 5.31: Experimentally measured temperature profiles for front east, front west, back east and back west SiC tubes.

The east/west temperature discrepancy is attributed to asymmetry in the flux profile resulting from the off-axis design of the HFSF. Individual simulations for east and west sides of the receiver suggest that the east side temperature exceeds the west by at most 60-70 K with a 6 kW solar input. Experimentally determined east/west temperature discrepancies range from 20-100 K for 1-4 kW solar power. Adjustments to the secondary concentrator position were unavoidable over the duration of experimentation and the resultant variability in alignment

renders comparison between theoretically predicted and experimentally measured asymmetry challenging. Adjustment of the secondary concentrator prior to measurement at the two highest power levels appears to skew the solar beam toward the west side of the receiver thereby reducing the east/west disparity.

Figure 5.32 provides analogous comparisons between theoretical predictions and experimental measurements for Inconel 600 tubes.



Figure 5.32: Experimentally measured temperature profiles for Inconel tubes compared with the theoretical model for (a) center tube (b) center and outer tubes

Experimental error for the measured temperature is provided by the standard deviation for replicate experiments at each power level. Systemic errors resulting from physical separation between the thermocouple and tube wall are quantified in Appendix E. Once again the theoretical model produces both qualitatively and quantitatively accurate predictions of the tube temperatures. Temperature measurements at the back of the center tube are unrealistically low because the thermocouple lost contact with the tube wall during experimentation. The average discrepancy between theory and experiment is 21 K or approximately 2% of the measured values neglecting the back wall. Figure 5.33 displays measured temperature for all four outer tubes and again indicates reproducible east/west symmetry attributed to the solar flux profile.



Figure 5.33: Experimentally measured temperature profiles for front east, front west, back east and back west Inconel tubes.

Inconel tubes produce higher maximum temperatures than silicon carbide tubes under identical operating conditions. This observation is substantiated by the theoretical model predictions and can be attributed to the thermal conductivity of the tube material which varies between 15-28 W/m/K and 120-60 W/m/K for Inconel 600 and Hexoloy SA SiC, respectively, as the temperature increases from 300-1100 K. The comparatively higher thermal conductivity of

silicon carbide allows for more effective heat transfer away from the heated region and toward the upper and lower cooling zones thereby diminishing peak temperatures in the horizontal center plane.

Heat losses measured for the top/bottom and front/back cavity wall cooling zones for both tube materials are shown in Table 5.22 alongside emission losses approximated by equation 5.94 as a fraction of solar energy incident on the window surface. Comparatively higher temperatures produced by Inconel tubes lead to increased energy loss by emission and absorption of emitted energy at the front and back cavity wall. Conversely, the comparatively higher thermal conductivity of silicon carbide results in increased loss by conduction along the tube length into the top and bottom cooling zones.

 Table 5.22: Comparison between experimental heat loss distributions for silicon carbide and Inconel tubes

	Silicon carbide	Inconel 600
Top/Bottom cooling zone	39-49%	26-32%
Front/back cooling zone	33-37%	42-47%
Emission	3.3-8.5%	7.6-13%

#### 5.9.4 Experimental validation for carbon gasification

Instantaneous measurement of solid feed rates is impractical during on-sun experimental testing and, as such, theoretical predictions are compared with measured values on the basis of average feed rate which varied between 0.26 mg/s and 0.40 mg/s. Total carbon conversion is determined from equation 5.95 where  $\bar{n}_c$  is the average molar feed rate of carbon,  $x_{CO}$  and  $x_{CO2}$  are, respectively, the measured molar fractions of CO and CO<sub>2</sub> in the effluent, and  $\dot{V}_s$  is the measured standard volumetric flow rate of the effluent.

$$X = \frac{1}{\bar{n}_{C}\Delta t} \int_{\Delta t} (x_{CO} + x_{CO2}) \frac{\dot{V}_{s} P_{s}}{RT_{s}} dt$$
(5.95)

The integral in equation 5.95 is carried out at steady state over a period of  $\Delta t = 5$  min. The resultant experimentally determined conversion of carbon to CO and CO<sub>2</sub> in the center tube is displayed in Figure 5.34 as a function of solar power.



Figure 5.34: Experimental measurement and theoretical predictions of carbon conversion to CO and  $CO_2$  in the center tube

The carbon particles are entrained in 0.75 SLPM of argon with an additional 0.25 SLPM sweep flow added separately at the tube inlet. The water feed rate is maintained at 108  $\mu$ L/min, three times the stoichiometric rate for 0.4 mg/s carbon. Experimental error is assessed assuming NDIR measurement uncertainty equal to 1% of the full range, or 100 ppm for each CO and CO<sub>2</sub>. Standard deviation between replicate experiments at the two highest power levels exceeds, and therefore replaces, this value. Uncertainty in the solar input is identical to that shown in Figure 5.30.

Curves from the theoretical model are generated with a tube inlet boundary condition modified from that described in section 5.6 for a more relevant comparison with experimental conditions. The modified boundary condition is detailed in Table 5.23. All carbon, steam, and

0.75 SLPM argon are introduced via a laminar flow profile (equation 5.80) with radius  $R_{inlet} = 0.32$  cm characterizing the inner feed tube. A uniform mass flux of 0.25 SLPM argon is applied between the inner region and the tube wall. Model predictions of fractional carbon conversion with carbon dispersed uniformly across the tube inlet exceed those generated with this modified boundary condition by as much as 0.02.

	$0 < r < R_{inlet}$	$R_{inlet} < r < R_{tube}$
Mass flux profile	Laminar flow	Uniform
$m_{C,0}$	0.4 mg/s	0
$F_{H2O,0}$	0.1343 SLPM	0
$F_{Ar,0}$	0.75 SLPM	0.25 SLPM
$W_{C,\theta}$	0.0315	0
W <sub>H2O,0</sub>	0.1889	0
$W_{Ar,0}$	0.7796	1

Table 5.23: Inlet boundary conditions for the carbon gasification model

Fifteen sets of kinetic parameters describing gasification of petcoke [11, 13, 58, 64, 74, 75], activated carbon [57, 76], graphite [77, 78], or low ash coal char [79] are taken from the literature and, in some cases, simplified to a first order model. Theoretical predictions of total carbon conversion using eight of these sets of kinetic parameters are illustrated in Figure 5.34 and identified by number in Table 5.24. The kinetic parameters in Table 5.24 are listed in the approximate order of highest to lowest carbon conversion predicted by the computational model at 5 kW solar power. The kinetic parameters produce a wide range of theoretically predicted carbon conversion perhaps owing to substantial variability in active surface area between materials or the influence of heat and mass transfer effects. The parameters given by Trommer et al. [64] produce line 3 in Figure 5.34 and appear to provide the closest match to experimental measurements.

Material	$k_o$ $(g/s/m^2/Pa)$	$E_a$	Line in Figure 5 34
graphite[77]	318	208.0	1 Iguit 5.54
petcoke [11]	248	218.6	2
petcoke [64]	5.60	186.6	3
petcoke [11]	0.498	161.5	4
activated charcoal [76]	14.6	205.3	5
petcoke [74]	123	238.0	6
petcoke [58]	0.977	181.2	-
petcoke [58]	0.161	161.8	-
petcoke [64]	4.03x10 <sup>-2</sup>	147.3	-
petcoke [13]	0.787	189.5	7
petcoke [64]	4.07x10 <sup>-4</sup>	128.8	-
low ash coal char [79]	6.28	227.0	-
petcoke [75]	1.26x10 <sup>-5</sup>	78.9	-
activated charcoal [57]	6.22x10 <sup>-2</sup>	182.0	-
graphite [78]	7390	337.0	8

Table 5.24: Literature values for kinetic parameters describing the steam gasification reaction

### 5.10 Conclusions

A theoretical model is developed for gasification of nano-sized acetylene black particles in a reflective cavity solar receiver. Radiative energy is separated into two components: solar energy introduced at the aperture and energy emitted by heated surfaces within the receiver. Solar energy is directly mapped from a profile at the window surface onto all tube and cavity wall surfaces by means of a statistically-based Monte Carlo technique. Emitted energy is approximated with a finite volume radiation model solved simultaneously and on the same spatial mesh as a three dimensional steady state computational fluid dynamics (CFD) model describing the heat, mass, momentum, and chemical reaction processes occurring in the receiver. This approach retains both the computational accuracy of the Monte Carlo method for the solar component, and the compatibility of the finite volume technique with control volume based CFD methods for the emitted component which is strongly dependent on surface temperatures and, correspondingly, all convection and conduction phenomena occurring in the receiver. The overall strategy computationally decouples the solar radiation solutions from all heat and mass transport processes occurring in the receiver thereby enhancing computational efficiency.

The magnitude and directionality of solar energy impinging on the window surface is characterized by ray trace modeling of the High Flux Solar Furnace (HFSF) at the National Renewable Energy Laboratory (NREL). The shape of the flux profile is only a weak function of attenuator opening, but distributions of directions at which this energy strikes the window surface reveal a complex dependence on attenuator opening as the line of sight between the aperture and upper or lower primary concentrator facets becomes obscured at low solar power inputs. Solutions from the Monte Carlo model take the form of profiles of solar energy flux absorbed as a function of position on each surface. The center tube absorbs 33% of the total solar energy, more than double that absorbed by any of the outlying tubes, and discernible disparities between energy received on the east and west sides of the reactor arise from flux profile asymmetry due to the off-axis design of the HFSF. More than 90% of solar absorption occurs prior to reflection. A finite volume model is utilized to account for energy emitted into the non-participating medium enclosed in the cavity space and the absorbing, emitting, and scattering fluid/particle mixture contained within the tubes. Absorption and scattering efficiency for 42 nm acetylene black particles are calculated from Mie theory and the resulting extinction coefficient is unmistakably dominated by absorption. Internal particle heat and mass transfer processes occurring during the gasification reaction are neglected as calculated effectiveness factors exceed 99.9%. Momentum and thermal Stokes numbers are on the order of  $10^{-5}$  implying

equivalent temperature and velocity for fluid and particulate phases. Given these assumptions an Eulerian-Eulerian two-fluid model is simplified to a single fluid mixture model with an aerosol population balance incorporating particle transport by convection, Brownian motion, and thermophoretic diffusion

Predicted temperatures exceed 1800 K with a solar power input of 6 kW but are highly non-uniform, particularly at the front of the center tube where temperature may vary by 450 K over a mere 5 cm of tube length. Front and back wall temperatures differ by as much as 350 K while fluid/particle temperature at the tube centerline tracks closely with surface temperatures owing to the influence of radiative heating. Maximum temperatures of 1813 K, 1343 K, and 1546 K are predicted for the center, front, and back tubes, respectively, with corresponding reaction conversions of 40.4%, 2.5%, and 9.2% for 6 kW solar power. Estimated receiver efficiency ranges between 1-4% depending of operating conditions. Low reaction conversion in the outlying tubes severely limits receiver efficiency as net absorption by these tubes accounts for 45% of the solar input, but each outlying tube fails to achieve temperatures high enough to carry out the gasification reaction to a significant extent. Reflection and absorption of solar energy by cooled surfaces account for 18-22% of the solar input. Emission losses, including absorption by actively cooled cavity walls, increase monotonically with solar input and account for 11-25% of the incident energy. Convective and conductive heat losses comprise 55-69% of the solar input and are predominantly attributed to conduction of absorbed energy along the length of the tubes to the upper and lower cooling zones. Average residence time is on the order of 1 s, but more than 80% of carbon conversion occurs within less than 15% of the tube length in a region where fluid velocity is maximized signifying that residence time in the heated length is a mere fraction of the total residence time. Model results are markedly more sensitive to

variability in physical and optical properties related to solid materials, particularly cavity wall reflectivity and tube thermal conductivity, than to variability in fluid properties. Alteration of individual input parameters by  $\pm 15\%$  produces at most a 60 K increase in temperature, a 0.06 increase in the fractional carbon conversion, and a 0.015 increase in the fractional receiver efficiency. Thus reasonable uncertainty in high temperature material properties is not enough to substantially improve the assessment of receiver performance.

Results from the numerical model are experimentally validated by comparison with reaction conversion and temperature profiles measured on-sun in the existing receiver. Temperature profiles are evaluated for both a metallic (Inconel 600) and ceramic (silicon carbide) tube material over temperature ranges of, respectively, 700-1400 K and 600-1700 K. The average discrepancies between theoretically predicted and experimentally measured temperatures are 44 K (4%) for silicon carbide and 21 K (2%) for Inconel. Relative distributions between heat loss mechanisms are directly comparable to those predicted from the theoretical model.

### Nomenclature

$a_i$	emissivity weighting factor in WSGG model
$a_{\lambda}$	spectral absorption coefficient (m <sup>-1</sup> )
$A_p$	geometric particle cross-sectional area (m <sup>2</sup> )
$A_{s,f}$	surface area of control volume face $f(m^2)$
$\hat{A}_s$	specific particle surface area (m <sup>2</sup> /kg)
С	concentration (mol/m <sup>3</sup> )
$C_c$	Cunningham correction factor
$C_p$	heat capacity (J/kg/K)
$C_{th}$	thermophoretic velocity (m/s)
$d_m$	gas molecular collision diameter (m)

$d_p$	particle diameter (m)
$d_{p0}$	initial particle diameter (m)
D	diffusivity (m <sup>2</sup> /s)
$D_e$	effective diffusivity (m <sup>2</sup> /s)
$E_a$	activation energy (J/mol)
f	forward scattering factor
$f_{gap}$	fraction of energy at the exit of secondary concentrator lost in the gap between the
	concentrator and receiver window surface
$f_{s,refl,cav}$	fraction of solar energy incident on the receiver window that is lost by reflection inside the receiver
$f_{s,refl,wind}$	fraction of solar energy incident on the receiver window that is lost by reflection at
	the external window surface
$f_v$	volume fraction
F	fluid volumetric flow rate (SLPM)
$F_{i-j}$	radiation configuration factor between surfaces <i>i</i> and <i>j</i>
g	gravitational acceleration (m/s <sup>2</sup> )
g'	asymmetry factor
h	enthalpy (J/kg)
	convective heat transfer coefficient $(W/m^2/K)$
Ι	identity matrix
$I_{\lambda}$	spectral radiation intensity between (W/m <sup>2</sup> /sr/µm)
$I_{\lambda b}$	spectral blackbody radiation intensity between (W/m <sup>2</sup> /sr/µm)
k	thermal conductivity (W/m/K)
	extinction coefficient
	reaction rate constant
$k_i$	absorption coefficient of the $i^{th}$ gray gas (W/m/K)
$k_{i0}$	pre-exponential factor
$k_B$	Boltzmann constant (kg $m^2/s^2/K$ )
$k_s$	intrinsic surface reaction rate constant on an area basis (kg/m <sup>2</sup> /Pa/s or m/s)
K <sub>eq</sub>	equilibrium constant
l	index denoting finite solid angle

т	mass flow rate (kg/s)
М	molecular weight
$M_{jk}$	interphase momtentum transport (kg/m <sup>2</sup> /s <sup>2</sup> )
n	index of refraction
n <sub>angle</sub>	number of divisions in each angle for flux profile specification
n <sub>c</sub>	molar flow rate of carbon (mol/s)
$n_f$	molar fluid flow rate (mol/s)
$\vec{n}_f$	surface normal vector for control volume face $f$
$\hat{n}_p$	mass-based particle number concentration (kg <sup>-1</sup> )
$N_f$	number of faces on control volume
$N_p$	number of particles per unit volume (m <sup>-3</sup> )
$N_{ heta}$	number of divisions of angle $\theta$ in the finite volume model
$N_{\theta p}$	number of pixels for angle $\theta$ in the finite volume model
$N_{arphi}$	number of divisions of angle $\varphi$ in the finite volume model
$N_{\varphi p}$	number of pixels for angle $\varphi$ in the finite volume model
р	pressure (Pa)
$P_n$	associated Legendre polynomials
q "abs,solar	absorbed solar flux (kW/m <sup>2</sup> )
q"inc,solar	incident solar flux (kW/m <sup>2</sup> )
q", <sub>,avg</sub>	average energy flux (kW/m <sup>2</sup> )
$\vec{q}_r$	radiative flux vector (W/m <sup>2</sup> )
$Q_{i,k}$	interphase energy transport (W/m <sup>3</sup> )
$Q_{abs}$	absorption efficiency
$Q_{sca}$	scattering efficiency
$Q_{conc}$	solar energy exiting the secondary concentrator (kW)
$Q_{cond}$	energy lost in cooling zones surrounding the receiver (kW)
$Q_{gap}$	solar energy lost between secondary concentrator and receiver window (kW)
$Q_{nom}$	solar energy entering the secondary concentrator (kW)
$Q_{re-rad}$	energy lost by re-radiation (kW)
$Q_{s,refl,cav}$	solar energy lost by reflection inside receiver (kW)

$Q_{s,refl,wind}$	solar energy lost by reflection at external window surface (kW)
$Q_{wind}$	solar energy incident on external window surface (kW)
$\vec{r}$	vector denoting spatial position
	vector between control volume centroid and face centroid
R	gas constant (J/kg/K)
$R_p$	particle radius (m)
$R_s$	surface reaction rate (kg/m <sup>2</sup> /s)
$R_{\nu}$	volumetric reaction rate (kg/m <sup>3</sup> /s)
$\vec{S}$	vector denoting radiation direction
S	coordinate along radiative energy path
	energy (W/m <sup>3</sup> ) or species (kg/m <sup>3</sup> /s) source term
Т	temperature (K)
$T_{ext}$	temperature of external surfaces (K)
$T_{rad}$	radiation temperature (K)
$T_{ref}$	reference temperature (K)
V	volume (m <sup>3</sup> )
$\dot{V_s}$	standard volumetric flow rate
Wi	mass fraction of species i
$x_i$	mole fraction of species i
X	carbon gasification reaction conversion
a	volume fraction
ß	angle around tube circumference measured from the direction facing the window
ף זי	angle measured from vertical axis to describe ray direction at aperture
r E	emissivity
n	receiver efficiency
'1	narticle reaction effectiveness factor
θ	zenith angle in global coordinate system
~	angle between incident and scattered directions
	incident angle relative to surface normal
2	wavelength
	·····

	gas mean free path (m)
μ	viscosity (kg/m/s)
ξ	particle size parameter
	moles of gas generated per mole solid reacted
ξn	Riccati-Bessel function
ρ	reflectivity
	density (kg/m <sup>3</sup> )
σ	Stefan-Boltzmann constant $(W/m^2/K^4)$
$\sigma_c$	collision diameter (Å)
$\sigma_{\lambda}$	spectral scattering coefficient (m <sup>-1</sup> )
τ	transmissivity
	tortuosity
$\vec{ au}$	viscous stress tensor (kg/m/s <sup>2</sup> )
$\vec{\upsilon}$	velocity (m/s)
$\varphi$	azimuth angle in global coordinate system
	Thiele modulus
Ψ	porosity
ω	discrete solid angle
	angle measured from horizontal axis to describe ray direction at aperture
$\Gamma_k$	interphase mass transport (kg/m <sup>3</sup> /s)
$\Delta H$	enthalpy of reaction
$\Phi$	scattering phase function
$\Psi_n$	Riccati-Bessel function
${\it \Omega}$	collision integral

## Subscripts and superscripts

avg	average
b	blackbody
	reverse (reaction)
	back
В	back tube

С	carbon
е	effective
ext	external
Ε	east side of receiver
f	index denoting control volume face
	forward (reaction)
	front
F	front tube
g	gas phase
in	inlet
l	index denoting finite discrete solid angle
т	medium
max	maximum
0	initial or inlet
out	outlet
р	index denoting control volume or centroid of control volume
	index denoting pixel
	particle phase
rad	radiation
ref	reference
S	surface
W	wall or boundary surface
	window
W	west side of receiver
v	volumetric
λ	spectral

# References

1. Kodama, T., High-temperature solar chemistry for converting solar heat to chemical fuels. *Progress in Energy and Combustion Science*, 2003. **29**(6): p. 567-597.

- 2. Kodama, T. and Gokon, N., Thermochernical cycles for high-temperature solar hydrogen production. *Chemical Reviews*, 2007. **107**(10): p. 4048-4077.
- 3. Steinfeld, A., Solar thermochemical production of hydrogen a review. *Solar Energy*, 2005. **78**(5): p. 603-615.
- 4. Abanades, S., Charvin, P., and Flamant, G., Design and simulation of a solar chemical reactor for the thermal reduction of metal oxides: Case study of zinc oxide dissociation. *Chemical Engineering Science*, 2007. **62**(22): p. 6323-6333.
- 5. Lichty, P., Perkins, C., Woodruff, B., Bingham, C., and Weimer, A., Rapid High Temperature Solar Thermal Biomass Gasification in a Prototype Cavity Reactor. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(1).
- 6. Melchior, T., Perkins, C., Weimer, A.W., and Steinfeld, A., A cavity-receiver containing a tubular absorber for high-temperature thermochemical processing using concentrated solar energy. *International Journal of Thermal Sciences*, 2008. **47**(11): p. 1496-1503.
- 7. Palumbo, R., Keunecke, M., Moller, S., and Steinfeld, A., Reflections on the design of solar thermal chemical reactors: thoughts in transformation. *Energy*, 2004. **29**(5-6): p. 727-744.
- 8. Siegel, N.P., Ho, C.K., Khalsa, S.S., and Kolb, G.J., Development and Evaluation of a Prototype Solid Particle Receiver: On-Sun Testing and Model Validation. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(2).
- 9. Steinfeld, A. and Fletcher, E.A., A Solar Receiver-Reactor with Specularly Reflecting Walls for High-Temperature Thermoelectrochemical and Thermochemical Processes. *Energy*, 1988. **13**(4): p. 301-311.
- 10. Wieckert, C., Palumbo, R., and Frommherz, U., A two-cavity reactor for solar chemical processes: heat transfer model and application to carbothermic reduction of ZnO. *Energy*, 2004. **29**(5-6): p. 771-787.
- 11. Z'Graggen, A. and Steinfeld, A., Hydrogen production by steam-gasification of carbonaceous materials using concentrated solar energy V. Reactor modeling, optimization, and scale-up. *International Journal of Hydrogen Energy*, 2008. **33**(20): p. 5484-5492.
- Haussener, S., Hirsch, D., Perkins, C., Weimer, A., Lewandowski, A., and Steinfeld, A., Modeling of a Multitube High-Temperature Solar Thermochemical Reactor for Hydrogen Production. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2009. 131(2).
- 13. Z'Graggen, A. and Steinfeld, A., A two-phase reactor model for the steam-gasification of carbonaceous materials under concentrated thermal radiation. *Chemical Engineering and Processing*, 2008. **47**(4): p. 655-662.

- 14. Hirsch, D. and Steinfeld, A., Radiative transfer in a solar chemical reactor for the coproduction of hydrogen and carbon by thermal decomposition of methane. *Chemical Engineering Science*, 2004. **59**(24): p. 5771-5778.
- 15. Maag, G. and Steinfeld, A., Design of a 10 MW Particle-Flow Reactor for Syngas Production by Steam-Gasification of Carbonaceous Feedstock Using Concentrated Solar Energy. *Energy & Fuels*, 2010. **24**: p. 6540-6547.
- 16. Chui, E.H. and Raithby, G.D., Computation of Radiant-Heat Transfer on a Nonorthogonal Mesh Using the Finite-Volume Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **23**(3): p. 269-288.
- 17. Raithby, G.D. and Chui, E.H., A Finite-Volume Method for Predicting a Radiant-Heat Transfer in Enclosures with Participating Media. *Journal of Heat Transfer-Transactions of the Asme*, 1990. **112**(2): p. 415-423.
- 18. Fiveland, W.A., Discrete Ordinate Methods for Radiative Heat-Transfer in Isotropically and Anisotropically Scattering Media. *Journal of Heat Transfer-Transactions of the Asme*, 1987. **109**(3): p. 809-812.
- 19. Byun, D.Y., Baek, S.W., and Kim, M.Y., Thermal radiation in a discretely heated irregular geometry using the Monte-Carlo, finite volume, and modified discrete ordinates interpolation method. *Numerical Heat Transfer Part a-Applications*, 2000. **37**(1): p. 1-18.
- 20. Chai, J.C., Lee, H.S., and Patankar, S.V., Ray Effect and False Scattering in the Discrete Ordinates Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **24**(4): p. 373-389.
- 21. Coelho, P.J., The role of ray effects and false scattering on the accuracy of the standard and modified discrete ordinates methods. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2002. **73**(2-5): p. 231-238.
- 22. Raithby, G.D., Evaluation of discretization errors in finite-volume radiant heat transfer predictions. *Numerical Heat Transfer Part B-Fundamentals*, 1999. **36**(3): p. 241-264.
- 23. Di Blasi, C., Combustion and gasification rates of lignocellulosic chars. *Progress in Energy and Combustion Science*, 2009. **35**(2): p. 121-140.
- 24. Dupont, C., Boissonnet, G., Seller, J.M., Gauthier, P., and Schweich, D., Study about the kinetic processes of biomass steam gasification. *Fuel*, 2007. **86**(1-2): p. 32-40.
- Lewandowski, A., Bingham, C., Ogallagher, J., Winston, R., and Sagie, D., Performance Characterization of the Seri High-Flux Solar Furnace. *Solar Energy Materials*, 1991.
   24(1-4): p. 550-563.
- 26. Dahl, J.K., Buechler, K.J., Weimer, A.W., Lewandowski, A., and Bingham, C., Solarthermal dissociation of methane in a fluid-wall aerosol flow reactor. *International Journal of Hydrogen Energy*, 2004. **29**(7): p. 725-736.

- 27. Wendelin, T. SolTRACE: A new optical modeling tool for concentrating solar optics. in *Proceedings of the ISEC: International Solar Energy Conference*. 2003. Kohala Coast, Hawaii: American Society of Mechanical Engineers.
- 28. Siegel, R. and Howell, J., *Thermal Radiation Heat Transfer*. 4 ed. 2002, New York: Taylor and Francis.
- 29. Murthy, J.Y. and Mathur, S.R., Finite volume method for radiative heat transfer using unstructured meshes. *Journal of Thermophysics and Heat Transfer*, 1998. **12**(3): p. 313-321.
- 30. Bohren, C.F. and Huffman, D.R., *Absorption and Scattering of Light by Small Particles*. 1983, New York: Wiley.
- 31. Joseph, J.H., Wiscombe, W.J., and Weinman, J.A., Delta-Eddington Approximation for Radiative Flux-Transfer. *Journal of the Atmospheric Sciences*, 1976. **33**(12): p. 2452-2459.
- 32. Crosbie, A.L. and Davidson, G.W., Dirac-Delta Function Approximations to the Scattering Phase Function. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1985. **33**(4): p. 391-409.
- Smith, T.F., Shen, Z.F., and Friedman, J.N., Evaluation of Coefficients for the Weighted Sum of Gray Gases Model. *Journal of Heat Transfer-Transactions of the Asme*, 1982. 104(4): p. 602-608.
- 34. Palik, E.D., ed. *Handbook of Optical Constants of Solids*. 1998, Academic Press: San Diego.
- 35. Touloukain, Y.S. and DeWitt, D.P., *Thermophysical Properties of Matter the TPRC Data Series*. Thermal radiative properties: metallic elements and alloys. Vol. 7. 1970, New York: Plenum Publishing.
- 36. Dalzell, W.H. and Sarofim, A.F., Optical Constants of Soot and Their Application to Heat-Flux Calculations. *Journal of Heat Transfer*, 1969. **91**(1): p. 100-104.
- 37. Ishii, M. and Hibiki, T., *Thermo-Fluid Dynamics of Two-Phase Flow*. 2006, New York: Springer Science-Business Media.
- 38. Ishii, M. and Mishima, K., 2-Fluid Model and Hydrodynamic Constitutive Relations. *Nuclear Engineering and Design*, 1984. **82**(2-3): p. 107-126.
- 39. Rosner, D.E. and Park, H.M., Thermophoretically Augmented Mass-Transfer Momentum-Transfer and Energy-Transfer Rates in High Particle Mass Loaded Laminar Forced-Convection Systems. *Chemical Engineering Science*, 1988. **43**(10): p. 2689-2704.
- 40. Bird, R.B., Stewart, W.E., and N., L.E., *Transport Phenomena*. 2 ed. 2002, New York: John Wiley and Sons, Inc.

- 41. Stratmann, F., Otto, E., and Fissan, H., Thermophoretical and Diffusional Particle-Transport in Cooled Laminar Tube Flow. *Journal of Aerosol Science*, 1994. **25**(7): p. 1305-1319.
- Walsh, J.K., Weimer, A.W., and Hrenya, C.M., Thermophoretic deposition of aerosol particles in laminar tube flow with mixed convection. *Journal of Aerosol Science*, 2006. 37(6): p. 715-734.
- 43. Hinds, W.C., *Aerosol Technology*. 1982, New York: John Wiley and Sons.
- 44. Poling, B.E., Prausnitz, J.M., and O'Connel, J.P., *The Properties of Gases and Liquids*. 5th ed. 2001, New York: McGraw-Hill.
- 45. Fuller, E.N., Schettle.Pd, and Giddings, J.C., A New Method for Prediction of Binary Gas-Phase Diffusion Coeffecients. *Industrial and Engineering Chemistry*, 1966. **58**(5): p. 19.
- 46. Incropera, F.P. and Dewitt, D.P., *Fundamentals of Heat and Mass Transfer*. 5th ed. 2002, New York: John Wiley and Sons.
- 47. Haynes, W.M., ed. *CRC Handbook of Chemistry and Physics*. 91st ed. 2010, CRC Press / Taylor and Francis: Boca Raton, FL.
- 48. Perry, R.H. and Green, D.W., eds. *Perry's Chemical Engineers' Handbook*. 7th ed. 1997, McGraw-Hill: New York.
- 49. Dawe, R.A. and Smith, E.B., Viscosity of Argon at High Temperatures. *Science*, 1969. **163**(3868): p. 675.
- 50. Degroot, W.F. and Richards, G.N., Relative Rates of Carbon Gasification in Oxygen, Steam and Carbon-Dioxide. *Carbon*, 1989. **27**(2): p. 247-252.
- 51. Laurendeau, N.M., Heterogeneous Kinetics of Coal Char Gasification and Combustion. *Progress in Energy and Combustion Science*, 1978. **4**(4): p. 221-270.
- 52. Mann, M.D., Knutson, R.Z., Erjavec, J., and Jacobsen, J.P., Modeling reaction kinetics of steam gasification for a transport gasifier. *Fuel*, 2004. **83**(11-12): p. 1643-1650.
- Bale, C., Chartrand, P., Degterov, S.A., Eriksson, G., Hack, K., Ben Mahfoud, R., Melancon, J., Pelton, A.D., and Petersen, S., FactSage thermochemical software and databases. *Calphad-Computer Coupling of Phase Diagrams and Thermochemistry*, 2002. 26(2): p. 189-228.
- 54. Barrio, M., Goble, B., Risnes, H., Henriksen, U., Hustad, J.E., and Sorensen, L.H., *Steam gasification of wood char and the effect oh hydrogen inhibition on the chemical kinetics*, in *Progress in thermochemical biomass conversion*, A. V. Bridgwater, Editor. 2001, Blackwell Science Ltd.: Oxford. p. 32-46.

- 55. Juntgen, H., Reactivities of Carbon to Steam and Hydrogen and Applications to Technical Gasification Processes a Review. *Carbon*, 1981. **19**(3): p. 167-173.
- 56. Muhlen, H.J., Vanheek, K.H., and Juntgen, H., Kinetic-Studies of Steam Gasification of Char in the Presence of H-2, Co2 and Co. *Fuel*, 1985. **64**(7): p. 944-949.
- 57. Muller, R., Von Zedtwitz, P., Wokaun, A., and Steinfeld, A., Kinetic investigation on steam gasification of charcoal under direct high-flux irradiation. *Chemical Engineering Science*, 2003. **58**(22): p. 5111-5119.
- 58. Trommer, D. and Steinfeld, A., Kinetic modeling for the combined pyrolysis and steam gasification of petroleum coke and experimental determination of the rate constants by dynamic thermogravimetry in the 500-1520 K range. *Energy & Fuels*, 2006. **20**(3): p. 1250-1258.
- Long, F.J. and Sykes, K.W., The Mechanism of the Steam-Carbon Reaction. *Proceedings* of the Royal Society of London Series a-Mathematical and Physical Sciences, 1948. 193(1034): p. 377-399.
- 60. Blackwood, J.D. and Mcgrory, F., The Carbon-Steam Reaction at High Pressure. *Australian Journal of Chemistry*, 1958. **11**(1): p. 16-33.
- 61. Fogler, H.S., *Elements of Chemical Reaction Engineering*. 3 ed. 1999, Upper Saddle River, New Jersey: Prentice Hall.
- 62. Johnson, J.L., Relationships between Coal-Char Gasification Reactivities and Physical and Chemical Coal and Coal-Char Properties. *Abstracts of Papers of the American Chemical Society*, 1975. **170**(Aug24): p. 30-30.
- 63. Walker, P.L., Foresti, R.J., and Wright, C.C., Surface Area Studies of Carbon-Carbon Dioxide Reaction. *Industrial and Engineering Chemistry*, 1953. **45**(8): p. 1703-1710.
- 64. Trommer, D., *Thermodynamic and Kinetic Analyses of the Solar Thermal Gasification of Petroleum Coke*. 2006, Swiss Federal Institute of Technology: Zurich.
- 65. Bhattacharya, A., Salam, L., Dudukovic, M.P., and Joseph, B., Experimental and Modeling Studies in Fixed-Bed Char Gasification. *Industrial & Engineering Chemistry Process Design and Development*, 1986. **25**(4): p. 988-996.
- 66. Biba, V., Macak, J., Klose, E., and Malecha, J., Mathematical-Model for Gasification of Coal under Pressure. *Industrial & Engineering Chemistry Process Design and Development*, 1978. **17**(1): p. 92-98.
- 67. Watanabe, H. and Otaka, M., Numerical simulation of coal gasification in entrained flow coal gasifier. *Fuel*, 2006. **85**(12-13): p. 1935-1943.

- 68. Bustamante, F., Enick, R.M., Cugini, A.V., Killmeyer, R.P., Howard, B.H., Rothenberger, K.S., Ciocco, M.V., and Morreale, B.D., High-temperature kinetics of the homogeneous reverse water-gas shift reaction. *Aiche Journal*, 2004. **50**(5): p. 1028-1041.
- 69. Bustamante, F., Enick, R.M., Killmeyer, R.P., Howard, B.H., Rothenberger, K.S., Cugini, A.V., Morreale, B.D., and Ciocco, M.V., Uncatalyzed and wall-catalyzed forward watergas shift reaction kinetics. *Aiche Journal*, 2005. **51**(5): p. 1440-1454.
- 70. Linstrom, P.J., and Mallard, W.G., NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, <u>http://webbook.nist.gov.</u>, ed.
- 71. Adanez, J. and Labiano, F.G., Modeling of Moving-Bed Coal Gasifiers. *Industrial & Engineering Chemistry Research*, 1990. **29**(10): p. 2079-2088.
- 72. Caram, H.S. and Amundson, N.R., Fluidized-Bed Gasification Reactor Modeling .1. Model Description and Numerical Results for a Single Bed. *Industrial & Engineering Chemistry Process Design and Development*, 1979. **18**(1): p. 80-96.
- Sudiro, M., Pellizzaro, M., Bezzo, F., and Bertucco, A., Simulated moving bed technology applied to coal gasification. *Chemical Engineering Research & Design*, 2010. 88(4A): p. 465-475.
- 74. Harris, D.J. and Smith, I.W., Intrinsic Reactivity of Coke and Char to Carbon-Dioxide. *Abstracts of Papers of the American Chemical Society*, 1989. **197**: p. 44-Fuel.
- 75. Trommer, D., Noembrini, F., Fasciana, A., Rodriguez, D., Morales, A., Romero, M., and Steinfeld, A., Hydrogen production by steam-gasification of petroleum coke using concentrated solar power I. Thermodynamic and kinetic analyses. *International Journal of Hydrogen Energy*, 2005. **30**(6): p. 605-618.
- 76. von Zedtwitz, P. and Steinfeld, A., Steam-gasification of coal in a fluidized-bed/packedbed reactor exposed to concentrated thermal radiation-modeling and experimental validation. *Industrial & Engineering Chemistry Research*, 2005. **44**(11): p. 3852-3861.
- 77. Mayers, M.A., The rate of oxidation of graphite by steam. *Journal of the American Chemical Society*, 1934. **56**(7): p. 1879-1881.
- Otto, K., Bartosiewicz, L., and Shelef, M., Catalytic Steam Gasification of Graphite -Effects of Calcium, Strontium, and Barium with and without Sulfur. *Carbon*, 1979. 17(4): p. 351-357.
- 79. Roberts, D.G. and Harris, D.J., Char gasification with O-2, CO2, and H2O: Effects of pressure on intrinsic reaction kinetics. *Energy & Fuels*, 2000. **14**(2): p. 483-489.

## **Chapter VI**

# Optimization studies for a multiple tube solar receiver based on combined radiation and computational fluid dynamics modeling: Reflective cavity

## 6.1 Abstract

An experimentally validated three-dimensional, steady state computational model coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics for steam gasification of acetylene black is utilized to investigate the impact of parameters describing operating conditions and tube configurations on the solar-to-chemical efficiency of a reflective cavity multiple-tube solar receiver. Geometric parameters are defined relative to a base design in which all tubes are arranged in a semicircle around the back cavity wall and allow for variations in cavity size, and number, radius, and arrangement of tubes with both staggered and non-staggered arrangements considered along with factors allowing for offset of all or part of the tube semicircle toward the aperture. Calculations indicate that maximizing the net absorption efficiency and minimizing emission losses are not an effective means of improving receiver performance; however, maximizing utilization of absorbed energy via minimization of tube conduction losses is essential. Thus delivering energy to the tube array in a manner conducive to energy utilization is of greater consequence than maximizing the net quantity of energy supplied to the tubes. Optimal designs allow a portion of the solar energy to reflect off of the cavity wall and typically contain three moderately sized tubes clustered near the back cavity wall and placed within the solar beam. Tubes positioned outside of the solar beam fail to achieve temperatures sufficient to reach high conversion of the endothermic gasification reaction. These outlying tubes instead act as heat sinks and contribute heavily to conductive losses. Calculation results indicate that reflective cavity receivers accepting up to 8 kW solar power may achieve efficiency as high as 13%. Constraints on the maximal allowable absorbed solar flux reduce the physically realistic receiver efficiency to 12.3%. Enhanced efficiency over the existing reflective cavity design stems principally from greater uniformity in absorbed energy and temperature distributions, longer heated tube length, and diminished conductive heat losses.

#### **6.2 Introduction**

Numerous solar reactor concepts have been proposed for high temperature thermochemical processes with most consisting of cavity-receiver type designs in which concentrated solar radiation enters into a closed cavity through a small aperture or window [1-8]. However, these receivers are generally designed with little fundamental basis leading to inadequacies including low efficiency and highly non-uniform heating. Receiver efficiency for designs scaled to accept up to 10 kW solar power typically ranges from 1-10% [8-15]. It is estimated that the optical components of the solar concentration system can account for as much as 50-80% of initial plant capital costs [16], and thus optimization of process economics is intrinsically tied to optimization of solar energy utilization within the receiver.

Various computational studies have investigated variability in receiver efficiency produced by linearly scaling a fixed geometry from 5-10 kW to 1-10 MW [8, 12, 15, 17, 18], but only a limited number of studies described in the literature have explored the impact of cavity size, tube configuration, and operating conditions on receiver efficiency at a fixed scale. Tescari et al. examined a receiver in which reactive material affixed around vertical cylindrical walls was heated via direct absorption of solar energy introduced at the top end of the cylinder [19, 20]. The impact of a shape factor and cylinder void fraction were investigated by means of a

constructal optimization method intended to approximate the tendency of geometric variations in the realistic system based on that predicted for a substantially simplified problem. Optimal efficiency for a uniform reactive material distribution was achieved with a small length to height ratio or shape factor. However, efficiency increased monotonically with shape factor when the quantity of reactive material decreased with increasing distance from the aperture.

Melchior et al. examined radiative transfer and surface temperature profiles in a perfectly insulated absorbing cavity receiver containing an array of one, two, four, or eight tubes via a Monte Carlo radiation model combined with macroscopic surface energy balances neglecting convective and conductive heat transfer [21]. The most uniform temperature distribution at the surface of a single tube occurred when the tube was positioned at 60% of the maximum distance from the aperture. Geometric spatial arrangement of the four or eight cylinders comprising the tube array ranged from a square shape to a straight line and produced no noteworthy effect on average array temperature despite substantial shadowing in certain configurations. The number of tubes had minimal impact on the average absorber temperature, though the optimal ratio of absorber radius to cavity radius shifted to lower values as the number of tubes increased.

Haussener et al. predicted the solar-to-chemical efficiency of a multiple tube receiver with an absorbing insulated cavity wall for thermal reduction of ZnO via a combined computational fluid dynamics and finite volume radiation model solved in a horizontal twodimensional slice of the receiver with a simplified heat sink representing chemical and sensible enthalpy requirements [22]. Receiver performance was evaluated with respect to solar concentration, number of tubes, tube size, and ZnO feed rate, and optimal receiver efficiency occurred at high solar concentration with a high ZnO feed rate distributed between a large number of tubes.

In the current study optimization calculations for the solar-to-chemical receiver efficiency are carried out via the experimentally validated three-dimensional, steady state computational model described in Chapter 5 coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics for steam gasification of acetylene black. This model provides a more physically realistic depiction of transport processes, temperature distributions, and chemical reaction kinetics than those employed in previous optimization studies. Sets of parameters describing receiver geometry and operating conditions are investigated by means of a series of fractional factorial design studies. These studies are applied as screening designs in order to identify parameters having substantial impact on receiver efficiency, and to ascertain approximate parameter ranges leading to ideal receiver performance. As the simulation results are not subject to random error, statistical significance of effects is not applicable and all parameters are evaluated purely based on relative effect magnitudes. All fractional factorial designs are chosen to be, at minimum, resolution IV implying that main effects are aliased solely with tertiary interactions or higher [23]. These high-order interactions are neglected on account of the sparsity of effects principle [23] thereby allowing estimation of main effects free from aliasing. A subset of significant parameters is examined in detail through a central composite design, and optima in the receiver efficiency are identified from the corresponding second-order response surface model.

## 6.3 Receiver configurations and computational model

#### 6.3.1 Receiver model

The experimentally validated computational model for heat, mass, momentum, chemical reaction, and radiation phenomena occurring in the reflective cavity receiver is described

comprehensively in Chapter 5. Calculations are carried out only for reactor configurations receiving up to 8 kW of solar energy with an aperture size identical to that of the existing receiver depicted schematically in Figure 1.1. The flux profile at the quartz window surface is that produced by the High Flux Solar Furnace (HFSF) at the National Renewable Energy Laboratory (NREL) as detailed in Chapter 5. All calculations are carried out with the ray directions and flux profile shape generated assuming an attenuator opening of 50%, and flux values are scaled linearly to yield the desired total power. The Monte Carlo model with spectral and directional optical properties described in Chapters 3 and 5 is utilized to produce profiles of absorbed solar energy flux as a function of spatial position on each surface in the receiver. These profiles are input into a three-dimensional steady state computational fluid dynamics (CFD) model which is solved simultaneously and on the same spatial mesh as a finite volume (FV) model for radiative energy emitted by heated surfaces. Given the elevated temperatures necessary to achieve sufficient reaction conversion, the preferred tube material is silicon carbide. All calculations in this study are carried out with spatial mesh elements sized similarly to those producing a grid-independent solution for the existing receiver configuration in Chapter 5. Finite solid angle extents are specified as described in Chapters 4 and 5 by  $N_{\theta} = N_{\Phi} = 7$ . A constant external wall temperature of 300 K is imposed at all reflective surfaces and laminar flow inlet profiles at 300 K are stipulated at the inlet of each tube. All combined CFD / FV models are solved in half of the symmetric geometry utilizing the Monte Carlo solution for solar radiation absorbed by the east side of the receiver.

Receiver configurations are evaluated for steam gasification of 42 nm carbon particles. Gasification kinetic parameters from Trommer et al. [24] produced superior predictions of experimental data and thus are used throughout this study. Solar-to-chemical efficiency of the multiple tube receiver is defined in equation 6.1 as the fraction of the incident solar power used to carry out the chemical reaction including sensible enthalpy requirements for the reactive components. Sensible enthalpy requirements for inert components or unconverted reactants are neglected.

$$\eta = \frac{\sum_{i}^{tubes} X_{C,i} \dot{n}_{Co,i} \Delta H_r(T_{avg,i}) + X_{C,i} \dot{n}_{Co,i} \int_{T_{inlet}}^{T_{avg,i}} (C_{p,C} + C_{p,steam}) dT}{Q_s}$$
(6.1)

In equation 6.1,  $X_{C,i}$  is the total carbon conversion in tube *i*, and  $\dot{n}_{Co,i}$  is the molar feed rate of carbon to tube *i*.  $T_{avg,i}$  is defined as the mass averaged fluid temperature in tube *i* at the horizontal center plane aligned with the aperture centroid and is computed using equation 6.2.

$$T_{avg,i} = \frac{\iint T\rho \left| \vec{\upsilon} \cdot d\vec{A} \right|}{\iint \rho \left| \vec{\upsilon} \cdot d\vec{A} \right|}$$
(6.2)

#### 6.3.2 Specification of parameters describing receiver geometry and operating conditions

Poor performance exhibited by the existing receiver largely stems from a discrepancy in solar energy absorbed between the individual tubes. The center tube absorbs two to four times more solar energy than the outer tubes leading to highly non-uniform temperature and reaction conversion profiles. The outlying tubes fail to attain temperatures high enough to carry out the gasification reaction to any significant extent while the center tube temperature approaches the maximal operating temperature dictated by the tube material. Furthermore, the existing design positions the center tube near the focal point of the primary concentrator leading to excessive solar irradiation on a small spatial region and producing undesirably large temperature gradients with a short heated length. Given these limitations, it appears that the design may well be improved by increasing the distance between the tube array and the focal point thereby allowing

spreading of the solar beam in order to increase the heated length and produce a more homogeneous distribution of absorbed energy between tubes. Consequently, all designs in this study are created relative to a base design with a semicircular arrangement of tubes around the back cavity wall.

Four parameters describing receiver operating conditions are included in the calculations. These parameters are the solar power input ( $Q_s$ ), total carbon feed rate ( $C_{feed}$ ), molar ratio of steam to carbon feed rates ( $R_{steam}$ ), and inert gas flow rate. Particles are entrained in inert gas by means of a brush feeder prior to being swept into the reaction tubes and the parameter specifying inert gas flow rate ( $R_l$ ) is defined as the ratio of the flow rate at standard conditions to the tube volume in front of the window. This definition is intended to provide a mechanism by which the impact of residence time at constant carbon and steam feed rates can be assessed. Variations in the cavity radius ( $r_{cav}$ ) and height ( $h_{cav}$ ) are evaluated with respect to constant aperture dimensions. Spatial tube positions are characterized relative to a base design with a semicircular arrangement of tubes around the back cavity wall. Two methods are defined for specification of tube positions, with detailed calculations provided in Appendix C. Method A utilizes the eight parameters illustrated in Figure 6.1 and allows for variations in tube number, size, and position.



Figure 6.1: Overview of parameters describing tube positions (method A)

 $N_{max}$  represents the maximum number of tubes in the base design depicted in Figure 6.1. The base design positions tubes on a semicircle described by radius  $r_{o,max}$  with the outermost tubes centered at the endpoints of the semicircle as dictated by Figure 6.2. The coordinate system identified in Figure 6.2(c) is created purely for specification of tube positions and is not aligned with that used in either the Monte Carlo or computational fluid dynamics models.



Figure 6.2: Specification of parameters describing tube positions (method A)

Removal of the tubes at the end of the array is accomplished via the parameter  $A/A_{max}$ . Minimum distance between the cavity and outermost tube walls  $(d_w)$  is maintained constant at 1.8 cm (0.7 in) regardless of the number or size of tubes. Parameter  $f_r$  is defined as the ratio of the cross-sectional area of the center tube to that of any of the uniformly-sized outer tubes. The total carbon feed is distributed between tubes proportional to the cross-sectional area in order to

maintain a nominally uniform residence time at standard conditions. Tube positions are related to either an outer circle defined by radius  $r_o$  or an inner circle defined by radius  $r_i$  as shown in Figure 6.2(b) with the relative values of  $r_o$  and  $r_i$  controlled by factor  $f_i$ . Outer and inner circles contain identically sized tubes and the inner circle is generated by broadening the outer circle such that the tubes at the end of the array are maintained in a constant position and the tubes at the back of the cavity are moved inward toward the focal point. The entire tube semicircle radius can be decreased and correspondingly moved toward the center of the cavity via the parameter  $f_2$ which is defined as the ratio between the actual and maximum tube surface area per unit length. Parameters  $f_s$  and  $f_o$  allow the tube array to be staggered or offset toward the window. Equations describing tube coordinates and radii are provided in Appendix C.

The second method employed to specify tube positions (method B) utilizes factors defined identically to those in Figures 6.1 and 6.2 with the exception of  $f_1$  and  $A/A_{max}$  which are removed and replaced with factor  $\theta_c$  describing the angular extent of the tube array measured from the center of the cavity as shown in Figure 6.3. The distance  $d_t$  between individual tube walls along the tube circle is fixed and used to specify the maximum tube radius. Detailed calculations providing tube coordinates are given in Appendix C.



Figure 6.3: Additional factor  $\theta_c$  for tube positions specified by method B

## 6.4 Design 1

A resolution IV  $2^{13-8}$  fractional factorial design consisting of 32 simulations is exploited to investigate the four operating conditions and nine of the geometric parameters described in Figure 6.1. Tube positions are specified via method A and the factor  $f_r$  is omitted in the current design leading to tube arrays composed of uniformly-sized cylinders. Low and high factor levels are specified in Table 6.1. Design generators are F = ACE, G = BCE, H = ABC, J = CDE, K = ABCDE, L = ABE, M = ACD, and N = ADE. Main effects in the resulting design are aliased with tertiary interactions or higher whereas each binary interaction is aliased with four or five additional binary interactions. The resulting 32 receiver configurations and simulation results are provided in detail in Appendix D.

Tellective cavity							
Factor	Nama	Low	High				
Factor	Indiffe	level	level				
А	$N_{max}$	5	9				
В	$A/A_{max}$	0.6	1				
С	$f_{I}$	0	0.4				
D	r/r <sub>max</sub>	0.6	1				
Е	$f_2$	0.6	1				
F	$f_o$	0	0.15				
G	$f_s$	0	0.25				
Н	$r_{cav}$	3.6 in	6 in				
J	$h_{cav}$	8 in	14 in				
K	$C_{feed}$	2 g/min	6 g/min				
L	R <sub>steam</sub>	1	2				
М	$R_I$	1 s <sup>-1</sup>	2 s <sup>-1</sup>				
Ν	$Q_s$	4.8 kW	7.0 kW				

Table 6.1: Factor levels for Design 1 ( $2^{13-8}$  fractional factorial):

Calculated solar-to-chemical efficiency ranges from 0.002-6.4%. For a given geometry, efficiency is unavoidably restricted by both emission and solar reflection losses as well as by the

feed rate of carbon. These independent restrictions produce two separate calculations of the maximal achievable receiver efficiency:  $\eta_{max,rad}$  and  $\eta_{max,C}$ . Emission and reflection losses account for 12-28% of the total solar energy under the conditions specified in Table 6.1 and Appendix D. The maximum receiver efficiency for a given carbon feed rate  $(\eta_{max,C})$  occurs when all carbon is converted to CO or CO<sub>2</sub>. The resultant values for the operating conditions in Table 6.1 range from 7-34% and thus are clearly more restrictive than the maximal efficiency based on emission and reflection losses. The limiting value can be improved by scaling the carbon feed rate such that the energy requirement for the endothermic reaction matches the solar power input, but increased carbon feed rate comes at the expense of a shorter residence time and diminished reaction conversion. Table D.1 lists the maximum carbon conversion occurring in any given tube  $(X_{max})$ , the average conversion between all tubes in the receiver  $(X_{avg})$ , the maximum fluid temperature occurring in any tube  $(T_{max})$ , and the lowest maximum fluid temperature obtained in any tube  $(T_{min})$ . Maximum fluid temperature ranges from 1324-1988 K producing up to 51% carbon conversion, though average carbon conversion reaches at best 26%. The difference between  $T_{max}$  and  $T_{min}$  provides a metric by which temperature uniformity between tubes may be assessed and ranges from 110-690 K for the factor levels in Table 6.1.

The net absorption efficiency is calculated from equation 6.3 where  $q''_{i,solar,abs}$  is the solar energy flux absorbed by tube *i* as a function of position,  $q''_{i,IR,abs}$  is the emitted energy flux absorbed by tube *i*, and  $q''_{i,IR,emitted}$  is the energy flux emitted by tube *i*.

$$\eta_{abs,net} = \frac{\sum_{i=1}^{hoes} \iint_{A_{s,i}} q''_{i,solar,abs} \, dA + \iint_{A_{s,i}} q''_{i,IR,abs} \, dA - \iint_{A_{s,i}} q''_{i,IR,emitted} \, dA}{Q_s} \tag{6.3}$$

All integrals are evaluated in the computational fluid dynamics (CFD) model as summations over mesh element faces on the tube boundary and the net absorption efficiency ranges from 20-

78% for the conditions in Table 6.1. The overall efficiency can be broken down into two components as shown in equation 6.4: the ratio of the energy used for the reaction to the energy transferred into the tubes ( $\eta_1$ ), and the ratio of the energy transferred into the tubes to the total solar energy ( $\eta_2$ ).

$$\eta = \eta_1 \eta_2 = \frac{Q_{reaction}}{Q_{tubes}} \frac{Q_{tubes}}{Q_s}$$
(6.4)

The energy required for the endothermic reaction is provided by the numerator of equation 6.1 while the energy transferred into the tubes is calculated from the CFD model by means of equation 6.5 where  $q''_{i,in}$  is the energy flux transferred away from the outer surface of tube *i* and into the solid material. The corresponding values of  $\eta_2$  are typically similar to the net absorption efficiency as heating of the tubular array is accomplished predominantly by radiative transfer.

$$Q_{tubes} = \sum_{i=1}^{tubes} \iint_{A_{s,i}} q''_{i,in} \, dA \tag{6.5}$$

#### 6.4.1 Evaluation of effects

Table 6.2 provides the main effects and binary interactions calculated from the fractional factorial design described in Table 6.1 for both  $\eta$  and  $\eta/\eta_{max,C}$ . Binary interactions are identified based on the factor designation for the first of five or six binary interactions present in a given alias chain. Factors are ordered from highest to lowest effect magnitude for receiver efficiency. Variability in solar-to-chemical efficiency between designs is clearly dominated by cavity radius and solar power input as designs with large  $r_{cav}$  or low  $Q_s$  fail to reach sufficiently high temperatures to carry out the gasification reaction.

Effect		Effect		Effect				
	η	$\eta/\eta_{max,C}$		η	$\eta/\eta_{max,C}$		η	$\eta/\eta_{max,C}$
r <sub>cav</sub>	-1.75%	-9.83%	$f_s$	-0.43%	-2.77%	ABN	0.19%	0.75%
$Q_s$	1.18%	8.09%	$A/A_{max}$	-0.42%	-2.83%	AG	0.19%	1.24%
$C_{feed}$	0.99%	-1.73%	AB	0.38%	2.16%	r/r <sub>max</sub>	-0.15%	-1.15%
AH	0.85%	1.42%	AE	0.34%	2.24%	h <sub>cav</sub>	0.14%	-0.27%
AN	-0.74%	0.29%	AF	0.34%	1.47%	$f_o$	0.13%	0.45%
AK	-0.74%	-4.29%	$f_I$	-0.33%	-1.21%	BM	-0.11%	0.35%
N <sub>max</sub>	-0.70%	-2.22%	AC	0.31%	1.16%	AM	-0.10%	0.92%
$f_2$	-0.53%	-2.83%	BN	-0.21%	-0.81%	ABD	0.07%	-0.59%
$R_I$	-0.53%	-2.74%	BD	0.21%	0.46%	ABM	-0.06%	-1.32%
<b>R</b> <sub>steam</sub>	-0.46%	-2.52%	AL	-0.19%	0.28%	AD	-0.03%	0.85%
						AJ	0.02%	1.27%

Table 6.2: Effect magnitudes for Design 1 ( $2^{13-8}$  fractional factorial): reflective cavity

The most significant factors describing tube configuration are  $N_{max}$  and  $f_2$  with the efficiency, on average, increasing as the number of tubes in the receiver decreases or as the tubes are moved inward toward the center of the cavity. Both  $f_o$  and  $h_{cav}$  appear to have a negligible impact on the simulation results. Physical constraints stipulate that the offset of the tube array toward the aperture via factor  $f_o$  can only occur over a range that is likely too limited to observe any impact on receiver performance. The relative insignificance of the cavity height is to be expected given the uniform window dimensions. Calculation results in Chapter 5 indicate that the heated tube length is only slightly larger than the window surface and thus extending the comparatively cool tube regions does little to improve carbon conversion. Lengthening the tubes physically separates the hot zone from the upper and lower cooling zones and thus theoretically diminishes conductive losses while simultaneously augmenting emission losses. The results in Table 6.2 suggest that these two effects offset and produce no net impact on average conversion or receiver efficiency.

Various binary interactions appear among the parameters with the largest impact on efficiency in Table 6.2. The most significant, identified by their full alias structure up to tertiary interactions are: AH+BC+EG+FL+KN, AN+CJ+DE+FM+HK, and AK+BJ+DG+HN+LM. The convoluted alias structure present in this screening design prohibits identification of the exact nature of the interactions responsible for the observed effects. Yet given the relative magnitudes of the constitutive main effects it seems probable that the AH interaction results from either  $N_{max}$  and  $r_{cav}$  (AH) or  $C_{feed}$  and  $Q_s$  (KN). The average efficiencies at each treatment combination giving rise to this interaction are displayed in Table 6.3. The KN interaction implies that solar power has a stronger positive impact on efficiency at high carbon feed rates than low whereas the AH interaction indicates that efficiency decreases relatively more as cavity radius increases when the number of tubes in the array is minimized. The KN interaction has the most straightforward physical interpretation as the benefit of increased solar power can only be realized with a sufficiently high carbon feed rate. Given the relative magnitudes of the main effects, the AN interaction is likely due to the interaction between  $N_{max}$  and  $Q_s$  (AN),  $r/r_{max}$  and  $f_2$ (DE), or  $r_{cav}$  and  $C_{feed}$  (HK) whereas the AK interaction is likely due to the interaction between  $N_{max}$  and  $C_{feed}$  (AK) or  $r_{cav}$  and  $Q_s$  (HN).

K	$N\left(Q_{s} ight)$		Α	H (r <sub>cav</sub> )	
$(C_{feed})$	Low	High	$(N_{max})$	Low	High
Low	0.69%	1.08%	Low	3.29%	0.40%
High	0.83%	3.15%	High	1.52%	0.56%

Table 6.3: Average efficiency at treatment combinations involving  $C_{feed}$ ,  $Q_s$ ,  $N_{max}$ , and  $r_{cav}$ 

The impacts of each main effect and binary interaction on the ratio of the observed efficiency to the maximum achievable efficiency based on complete carbon conversion ( $\eta/\eta_{max,C}$ )
are also identified in Table 6.2. Note that  $\eta/\eta_{max,C}$  is approximately equivalent to the average conversion attained in the receiver. Increasing the carbon feed rate produces a higher maximum efficiency as more reactive material is available for conversion, but also results in diminished residence time and conversion as the corresponding steam flow rate must be increased proportionally to maintain a stoichiometric ratio of reactants. Excessively high carbon feed rates may inhibit radiative heat transfer to the center region of the tube as particles in this center region become shielded from the tube walls and must rely on successive absorption and emission from particles residing closer to the tube walls. These considerations combine to produce a net negative effect of carbon flow rate on average conversion and  $\eta/\eta_{max,C}$ . Though the magnitudes of each main effect and binary interaction are clearly different for  $\eta$  and  $\eta/\eta_{max,C}$ , the relative order of most to least significant effects remains essentially unchanged with the notable exception of main effects or binary interactions involving carbon feed rate. Both AH and AN interactions exhibit a smaller relative effect on  $\eta/\eta_{max,C}$  than on  $\eta$ , suggesting that the large effect on  $\eta$  is attributable to an interaction involving the carbon feed rate. Thus the AH and AN interactions are likely primarily due to  $C_{feed} / Q_s$  and  $C_{feed} / r_{cav}$  respectively. The AK interaction remains significant for  $\eta/\eta_{max,C}$  suggesting that the  $r_{cav}/Q_s$  interaction dominates over the  $C_{feed}/Q_s$  $N_{max}$  interaction.

Identification of significant parameters is complicated by the large spread in receiver efficiency arising from the 32 models. The combination of low  $Q_s$  and high  $r_{cav}$  severely limits tube temperatures and these low temperatures, coupled with low  $C_{feed}$ , place considerable restriction on attainable receiver efficiency regardless of tube configuration. Main effects are assessed purely from response averages at low and high factor levels and thus the presence of outlying results can skew factor evaluation. Figure 6.4 illustrates the calculated efficiency as a

function of  $N_{max}$ . All high efficiency designs are characterized by low  $N_{max}$ , but the large number of designs with  $\eta < 1\%$  pulls down the average efficiency at the low level such that the calculated effect of  $N_{max}$  is only -0.7%. As only receiver configurations capable of operation at high efficiency are of interest, potentially more information can be gleaned from examination of the highest efficiency designs than can be obtained from a standard analysis of the fractional factorial design. Design numbers 9, 17, and 15 shown in Figure D.1 in Appendix D produce solar-to-chemical efficiency of 6.4%, 5.1%, and 4.6% respectively. Each design contains three to five tubes positioned in the middle region of the reflective cavity with low  $r_{cav}$ , high  $Q_s$ , and high  $C_{feed}$ .



Figure 6.4: Effect of  $N_{max}$  on receiver efficiency from Design 1

#### 6.4.2. Relationship between responses

Equation 6.4 describes the breakdown of efficiency into two components: the ratio of the energy used for the reaction to the energy transferred into the tubes ( $\eta_1$ ), and the ratio of the energy transferred into the tubes to the total solar energy ( $\eta_2$ ). Figure 6.5 illustrates a clear linear relationship between  $\eta$  and  $\eta_1$  with a correlation coefficient of 0.95; however, no apparent relationship is evident between  $\eta$  and  $\eta_2$  with a correlation coefficient of only -0.31. Thus while providing energy to the tubes in a manner conducive to energy utilization is imperative to

improving receiver efficiency, maximizing the net quantity of energy supplied to the tubes appears to be of little consequence. An analogous relationship exists between  $\eta$  and  $\eta_{abs,net}$ though  $\eta_2$  is 5-10% lower than the net absorption efficiency defined in equation 6.3 due to the influence of convective and conductive heat transfer. Designs with high absorption efficiency are not necessarily those that produce optimal receiver efficiency. On the contrary, the highest receiver efficiency typically occurs when absorption efficiency is held at an intermediate value.



Figure 6.5: Receiver efficiency from Design 1 as a function of (a)  $\eta_1$  and (b)  $\eta_2$ 

Likewise, Figure 6.6 indicates that highly efficient designs allow a portion of the solar energy to strike and reflect off of the cavity wall. Figure 6.6 depicts the relationship between the calculated receiver efficiency and the solar energy absorption efficiency of the cavity wall. Cavity wall reflection can be utilized to redistribute solar energy in the cavity space, potentially directing a portion of the energy toward the back of the tube array thereby improving uniformity in the distribution of absorbed solar energy around each tube surface. While a uniform tube temperature distribution promotes higher gasification reaction conversion, a fraction of the solar energy is irretrievably lost by absorption and conduction through the actively cooled cavity wall

at each reflection. Thus only a moderate quantity of solar energy can realistically be allowed to strike the cavity wall while retaining high receiver efficiency.



Figure 6.6: Receiver efficiency from Design 1 as a function of cavity wall solar absorption efficiency

Figure 6.7 relates the receiver efficiency to the approximate tube residence time calculated from the simplified plug flow model detailed in section 5.7.5. Residence time in the heated tube length is substantially shorter than that calculated for the entire tube in Figure 6.7. Figure 6.7 reveals that the highest efficiency is achieved at relatively short residence time, and suggests that the short residence time alone is not to blame for inadequate receiver efficiency. This is partially an artifact of the high carbon feed rates required to match solar power input to reaction enthalpy, and the concomitant rapid steam flow rate necessary to maintain at least a stoichiometric ratio of steam to carbon. Yet even designs with identically high  $C_{feed}$  exhibit the highest efficiency at short residence time.

Under these conditions efficiency increases nearly linearly with average carbon conversion ( $X_{avg}$ ), with separate linear relationships observed based on carbon feed rate shown in Figure 6.8(a). Thus improving average reaction conversion is critical to increasing receiver efficiency. This linear relationship can be deduced from the results in Table 6.2 indicating the

same sets of factors have a large impact on both efficiency and  $\eta/\eta_{max,C}$ . A slightly less clear trend is observed in the relationship between receiver efficiency and the maximum carbon conversion ( $X_{max}$ ) which typically occurs in the center tube. These results underscore the importance of improving conversion in the outer tubes as an increase in average conversion from 10-25% can lead to a 3.5% increase in receiver efficiency at high  $C_{feed}$ .



Figure 6.7: Receiver efficiency from Design 1 as a function of average plug flow residence time



carbon conversion

Principle mechanisms of heat loss are emission by the heated tube surfaces and conduction along the tube surfaces into cooling zones at the top and bottom of the receiver.

Emission losses can occur via transmission out of the window or absorption at actively cooled surfaces. Figure 6.9 relates the receiver efficiency to the fraction of solar energy lost by each mechanism and suggests that minimization of conduction losses is more essential than corresponding minimization of emission losses. Conduction losses tend to increase when designs contain tubes located in regions far removed from the solar beam as these tubes fail to reach temperatures high enough to carry out the reaction and instead function as heat sinks conducting energy away from the hot zone. Examination of the detailed results in Appendix D reveals that an increase in total tube surface area shifts the dominant mode of heat loss from emission to conduction as a greater number of tubes must be placed outside of the solar beam. Thus the preferred receiver configuration will restrict total tube area and place the tubes in the center region of the cavity such that a portion of the energy is allowed to strike the cavity wall. Though this configuration results in increased energy losses by emission owing to a larger tubeto-window view factor and minimal tube area for re-absorption of emitted energy, it also limits conduction losses as absorption is restricted to tubes capable of achieving high reaction conversion.



Figure 6.9: Relationship between efficiency from Design 1 and the fraction of energy lost by (a) emission and (b) conduction along tube length

## 6.5 Design 2

The results from Design 1 indicate that solar power, carbon feed rate, cavity radius and the maximum number of tubes all play a strong role in controlling receiver efficiency. However, evaluation of parameters describing receiver geometry is hindered by the poor receiver performance observed at low  $Q_s$ , low  $C_{feed}$ , and high  $r_{cav}$ , regardless of tube positions. Various binary interactions are noteworthy, though the exact nature of these interactions cannot be unambiguously distinguished due to a complex alias structure. As only receiver configurations producing high efficiency are of interest, the parameters describing receiver geometry are reevaluated under constant operating conditions. A resolution IV 2<sup>6-2</sup> fractional factorial design consisting of 16 simulations is used to investigate six of the parameters describing tube configurations with low and high factor levels specified in Table 6.4. Operating conditions and cavity radius are held constant at  $R_I = 1 \text{ s}^{-1}$ ,  $C_{feed} = 6 \text{ g/min}$ ,  $R_{steam} = 1$ ,  $Q_s = 7 \text{ kW}$ , and  $r_{cav} = 3.6$  in (9.14 cm). Tube positions are specified via method A with cavity height and offset of the tube array toward the aperture maintained at  $h_{cav} = 8$  in and  $f_o = 0$  based on the limited impact of these factors observed in Design 1.

Factor	Name	Low level	High level
А	$A/A_{max}$	0.6	1
В	r/r <sub>max</sub>	0.6	1
С	$N_{max}$	5	9
D	$f_l$	0	0.4
Е	$f_s$	0	0.25
F	$f_2$	0.6	1

Table 6.4: Geometric factor levels for Design 2 (2<sup>6-2</sup> fractional factorial): reflective cavity

Design generators are E = ABC and F = BCD. Main effects in the resulting design are aliased with tertiary or higher interactions whereas each binary interaction is aliased with at most one other binary interaction [23]. The resulting 16 receiver configurations and simulation results are provided in detail in Appendix D. Factor designations were altered from those in Table 6.1 so as to generate an entirely distinct set of tube configurations. Calculated receiver efficiency ranges from 1.9-7.2% while the maximal efficiency at complete carbon conversion ranges from 23-25% based on slight variations in average temperature. Net absorption efficiency, maximum carbon conversion, and maximum tube fluid temperature vary between 26-63%, 11-53%, and 1751-2034 K respectively.

### 6.5.1 Evaluation of effects

Table 6.5 presents the main effects and binary interactions calculated from the fractional factorial design described in Table 6.4 with factors ordered from high to low effect magnitude on receiver efficiency. These effect magnitudes differ from the corresponding values in Table 6.2 signifying non-negligible interactions between receiver geometry and operating conditions or cavity size. Effect magnitudes listed in Table 6.5 are evaluated exclusively at levels of operating conditions and  $r_{cav}$  producing superior receiver performance and are thus more relevant than those evaluated in Table 6.2.

	Effect		Effect
$A/A_{max}$	-1.76%	AB + CE	-0.43%
BF + CD	-1.27%	AD + EF	0.38%
N <sub>max</sub>	-1.22%	AC + BE	0.22%
BD + CF	0.93%	$f_l$	0.17%
r/r <sub>max</sub>	0.91%	$f_s$	-0.14%
AE + BC	0.89%	$f_2$	-0.14%
AF + DE	-0.84%		

Table 6.5: Effect magnitudes for Design 2 ( $2^{6-2}$  fractional factorial): reflective cavity

Variability in efficiency is dominated by main effects  $A/A_{max}$  and  $N_{max}$  with optimal receiver performance occurring for designs in which the outermost tubes are removed from the ends of the array. This behavior is consistent with results obtained from Design 1 in the previous section. As noted above, the outermost tubes fail to reach temperatures high enough to carry out the reaction and instead function as heat sinks conducting energy away from the hot zone. Utilization of low values of parameter  $A/A_{max}$  results in removal of the outermost tubes thereby allowing the energy that those tubes would have absorbed to reflect off of the cavity wall and reach the remaining tubes. Figure 6.10 illustrates the efficiency as a function of the number of tubes in the receiver and clearly reveals that, in accordance with main effects in Table 6.5, optimal configurations contain three tubes.



Figure 6.10: Receiver efficiency from Design 2 as a function of tube number

Based on the magnitude of constitutive main effects, it is likely that the notable binary interactions result from  $r/r_{max}$  and  $f_2$  (*BF*),  $N_{max}$  and  $f_2$  (*CF*),  $r/r_{max}$  and  $N_{max}$  (*BC*), and  $A/A_{max}$  and  $f_2$  (*AF*) rather than  $N_{max}$  and  $f_1$  (*CD*),  $r/r_{max}$  and  $f_1$  (*BD*),  $A/A_{max}$  and  $f_s$  (*AE*), and  $f_1$  and  $f_s$  (*DE*). Each of the *BF*, *CF*, *BC*, and *AF*, interactions has a physically realistic explanation. Response averages at each treatment combination are shown in Table 6.6

	B (r/	(r <sub>max</sub> )		C (1	V <sub>max</sub> )
$F(f_2)$	Low	High	$F(f_2)$	Low	High
Low	3.6%	5.8%	Low	5.8%	3.6%
High	4.8%	4.4%	High	4.7%	4.4%
В	C(N)	V <sub>max</sub> )		A (A/	$(A_{max})$
$(r/r_{max})$	Low	High	$F(f_2)$	Low	High
Low	5.3%	3.1%	Low	5.2%	4.3%
High	5.3%	4.9%	High	5.9%	3.3%

Table 6.6: Average efficiency at various treatment combinations from Design 2

Tube radii decrease as  $f_2$  and  $r/r_{max}$  decrease or as  $N_{max}$  increases. Thus the *BF* interaction implies that designs with smaller tubes (low  $f_2$ ) benefit greatly from increased tube radius (high  $r/r_{max}$ ) whereas those with larger tubes (high  $f_2$ ) benefit slightly from decreased tube radius (low  $r/r_{max}$ ). The *CF* and *BC* interactions imply that decreasing the maximum number of tubes and thereby increasing the tube size is most advantageous at low  $f_2$  and low  $r/r_{max}$ . All three interactions point toward an optimum intermediate tube radius with efficiency increasing as tube radius increases for initially small tubes and efficiency decreasing as tube radius increases for initially large tubes. The interaction between  $f_2$  and  $A/A_{max}$  implies that removing the tubes at the end of the array is most beneficial when  $f_2$  is high. Configurations characterized by low  $f_2$ position the outermost tubes closer to the solar beam and thus removing these tubes is not essential. The interaction between  $r/r_{max}$  and  $f_2$  is identified by the designation *DE* in Design 1 and is part of the alias chain including *AN* which was previously attributed to the  $N_{max} / Q_s$ interaction. The interactions identified by *AH* and *AK* in Table 6.2 do not correspond to any of the interactions in the left hand side of Table 6.5.

#### 6.5.2 Effect of tube radius

Figure 6.11 relates the calculated receiver efficiency to both tube radius and total absorber area per unit length and, as expected from the interactions identified above, clearly indicates an optimal intermediate value of each variable.



Figure 6.11: Relationship between efficiency from Design 2 and (a) tube radius or (b) total absorber area per unit length

The efficiency, maximum carbon conversion, average carbon conversion, the ratio of energy used for reaction to energy transferred into the tubes ( $\eta_1$ ), and the ratio of the energy transferred into the tubes to the total solar energy ( $\eta_2$ ) are evaluated in Table 6.7 for the three reactor configurations with cross sections identified in Figure 6.12 and design numbers corresponding to those in Table D.2 and Figure D.2 in Appendix D. Each configuration contains three tubes placed near the center of the cavity with tube radius increasing from left to right in Figure 6.12. Table 6.7 shows that, as observed in Figure 6.11(a), receiver efficiency proceeds through a maximum value as the absorber tube radius increases. Larger tubes absorb more solar energy (higher  $\eta_2$ ), but this energy is utilized less effectively within the tubes (lower  $\eta_1$ ). Both carbon

conversion in the center tube  $(X_{max})$  and the average carbon conversion  $(X_{avg})$  are highest at moderate tube radius.

		Geometry				
	1 9 3					
η	5.6%	6.6%	5.6%			
X <sub>max</sub>	42%	52%	40%			
X <sub>avg</sub>	22%	26%	23%			
$\eta_1$	21%	19%	12%			
$\eta_2$	26%	35%	47%			

Table 6.7: Comparison of receiver configurations with increasing tube radius



Figure 6.12: Receiver configurations corresponding to designs in Table 6.7

Figure 6.13 displays profiles of energy absorbed around the circumference of the center tube in a horizontal plane aligned with the aperture centroid as a function of angle  $\beta$ , with  $\beta = 0$  defined at the side of the tube facing the aperture. Solar energy absorption dominates total absorption of radiative energy at this central plane. Absorption of energy emitted by heated surfaces accounts for only 150-250 kW/m<sup>2</sup> as shown in Figure 6.13(b) whereas solar absorption can account for more than 1000 kW/m<sup>2</sup> under these conditions. The solar energy absorbed by the back side of the central tube after specular reflection at the cavity wall increases dramatically as the tube radius decreases and more cavity wall area is left exposed. Configurations with the

smallest tube radius exhibit solar absorption at the tube back greater than even that at the tube front.



Figure 6.13: Energy flux absorbed by the center tube in a horizontal plane aligned with the aperture centroid for the configurations in Figure 6.12

Figure 6.14 depicts profiles of temperature in the center tube fluid in the horizontal plane aligned with the aperture centroid as a function of horizontal position x with  $(x-x_0)/r_t = 1$  defined at the tube front and  $(x-x_0)/r_t = -1$  defined at the tube back. All temperatures are normalized to the maximum temperature occurring within the plane and reactor configurations are those illustrated in Figure 6.12. Configurations with relatively small tubes exhibit a back wall temperature higher that that at the front wall as expected from the profiles of absorbed solar energy in Figure 6.13. Despite radiative heating, the centerline fluid temperature lags behind the wall temperatures as a result of the rapid gas velocity from the laminar flow pattern at the tube centerline. In the limit of zero fluid velocity, the centerline temperature approaches a value intermediate to that attained at the front and back walls as carbon particles absorb energy emitted by the higher temperature wall and re-emit that energy toward the lower temperature wall. For large tube radius the centerline fluid temperature wall. For large tube radius the centerline fluid temperature wall and revelocity limit due to comparatively slow gas flow rates, but the temperature of the back wall and thus the

corresponding limiting centerline value are low. The elevated back wall temperature achieved with small tubes increases the limit for the stagnant case, but rapid gas flow resulting from the small tube radius impedes the approach to this limiting value. These competing effects produce an optimal intermediate tube radius and, not coincidentally, the design with the highest centerline fluid temperature in Figure 6.14 leads to the highest reaction conversion and receiver efficiency.



Figure 6.14: Center tube fluid temperature in the horizontal plane aligned with the aperture centroid for the configurations in Figure 6.12

Results from the receiver model in Chapter 5 indicate that heat transfer to the center of the fluid/particle mixture is accomplished primarily by radiative exchange between tube walls and entrained carbon particles. The mean radiation penetration distance is defined as the inverse of the average volumetric absorption coefficient for the fluid/particle mixture. The absorption coefficient is specified in Chapter 5 and is a complex function of particle size, volume fraction, and local fluid conditions. The average absorption coefficient is calculated from the CFD model leading to a mean penetration distance ( $l_m$ ) of 1 cm, 1.6 cm, and 2 cm for designs 1, 9, and 3 respectively. The resultant ratios of radiation penetration distance to tube radius are 2.4, 1.9, and 1.5 indicating that, even for the largest tubes, radiative transfer to the tube centerline is not

hampered by absorption at the outer edges. Thus while convective and conductive heat transfer to the center of the tube would be hindered by large tube radius, this is not the case for radiative transfer.

#### 6.5.3 Relationship between responses

Figure 6.15 illustrates a strongly positive correlation with a correlation coefficient of 0.87 between the receiver efficiency and the ratio of energy used for the reaction to energy transferred into the tubes ( $\eta_1$ ). Conversely, the correlation coefficient between the receiver efficiency and the fraction of the solar energy transferred into the tubes ( $\eta_2$ ) is only -0.08 implying that tube positional modifications resulting in improved absorption efficiency alone are not an effective means of enhancing receiver efficiency.



Figure 6.15: Receiver efficiency from Design 2 as a function of (a)  $\eta_1$  and (b)  $\eta_2$ 

Relationships between receiver efficiency and cavity wall solar absorption efficiency, average tube residence time, and maximum conversion are analogous to those depicted in Figures 6.6-6.8 and are not repeated here. The linear relationship between receiver efficiency and average carbon conversion is shown in Figure 6.16 to be even stronger than that illustrated in Figure 6.6

with a correlation coefficient exceeding 0.99 for the conditions considered here. This linear relationship may not be retained at carbon feed rates higher than those considered in Figures 6.8 or 6.16. While a positive correlation exists between efficiency and maximum conversion, the correlation coefficient is only 0.62. Thus, as indicated by the results from Design 1, improving reaction conversion in the outlying tubes is a more effective method of enhancing receiver efficiency than increasing conversion in the center tube alone.



Figure 6.16: Receiver efficiency from Design 2 as a function of average reaction conversion

# 6.6 Design 3

Results from the two fractional factorial design studies detailed above clearly indicate that the best tube configurations minimize the fraction of the carbon feed positioned outside of the concentrated solar beam and that receiver operating conditions strongly impact performance. In these studies, the only effective means of concentrating the carbon feed in the center region of the receiver was removal of the outermost absorber tubes. Alternatively, the outer tubes can be retained in place and a non-uniform distribution of carbon utilized such that the carbon feed rate for the center tube exceeds that for the outermost tubes. The center tube radius must be

correspondingly increased to maintain a nominally constant residence time at standard conditions. The parameter  $f_r$  is defined as the ratio of the center tube cross-sectional area to that of any of the identically-sized outer tubes and introduced into the optimization studies. Tube positions are again calculated from method A in Appendix C with parameters  $f_s$ ,  $f_o$ ,  $f_1$ , and  $h_{cav}$ held constant at their low values in Table 6.1 as these parameters failed to influence receiver performance in previous calculations. Parameters describing inert gas and steam flow rates are maintained at  $R_I = 1$  s<sup>-1</sup> and  $R_{steam} = 1$  as an increase above these levels produced a detrimental impact on receiver performance in previous calculations. The remaining eight parameters including  $f_r$  are evaluated in a resolution IV  $2^{8-4}$  fractional factorial design with low and high factor levels provided in Table 6.8. Though results from Design 2 unambiguously indicated optimal low values of  $A/A_{max}$  and  $N_{max}$ , these results required removal of outer tubes to preferentially concentrate the carbon feed in the solar beam. As the parameter  $f_r$  now provides an independent mechanism for accomplishing this goal, the  $A/A_{max}$  and  $N_{max}$  parameters are retained in the current design for comparison. This comparison allows for assessment of whether the design is best served by allowing energy to reflect off of the cavity wall after traveling through the empty space vacated by the outer tubes, or by allowing the outer tubes to function as radiant absorbers with minimal carbon feed rate. Designations of repeated geometric factors are kept identical to those in Table 6.4 to produce overlap in receiver configurations and reduce preprocessing effort. Design generators for the  $2^{8-4}$  fractional factorial design are E = BCD, F = ACD, G = ABC, and H = ABD. Calculations are carried out for both the range of  $Q_s$  shown in Table 6.8 and for  $Q_s = 7-8$  kW. To limit computational expense, factor levels for the high range of  $Q_s$  are coded such that 8 kW replaces 6 kW as the "low" level.

Factor	Name	Low level	High level
Α	$A/A_{max}$	0.6	1
В	r/r <sub>max</sub>	0.6	1
С	$A_{max}$	5	9
D	$f_r$	1	3
Е	$f_2$	0.6	1
F	$C_{feed}$	2 g/min	6 g/min
G	r <sub>cav</sub>	3.6 in	4.8 in
Н	$Q_s$	6 kW	7 kW

Table 6.8: Factor levels for Design 3 (2<sup>8-4</sup> fractional factorial): reflectivity cavity

Calculated receiver efficiency ranges from 0.4-8.4%, representing 4-39% or 4-54% of the efficiency at complete carbon conversion for solar inputs of, respectively, 6-7 kW or 7-8 kW. Maximum carbon conversion ranges from 7-58% or 7-75% and maximum temperature varies between 1530-1980 K or 1610-2170 K for, respectively, 6-7 kW or 7-8 kW. Note that the elevated power input raises temperatures above those reasonable for continuous operation of the silicon carbide tube material in an oxidizing environment. Furthermore, maximum solar energy flux absorbed at any point in the receiver increases from 474-1590  $kW/m^2$  for 6-7 kW to 570-2200 kW/m<sup>2</sup> for 7-8 kW. Localized tube cracking and material weakness are commonly encountered at the front of the center tube during on-sun experimental operation of the existing receiver with a solar power input exceeding 5.5 kW. Though the temperature at the inner tube surface is predicted to be less than 1700 K at this solar power input, calculations from the Monte Carlo model indicate an absorbed solar flux of 1100 kW/m<sup>2</sup> at the external tube surface. Material weakness may result from large localized temperature gradients occurring when conduction away from the tube surface is not rapid enough to distribute the absorbed energy, and thus it is desirable to restrict the maximum absorbed solar flux to values below  $1100 \text{ kW/m}^2$ .

This restriction places limitations on physically reasonable combinations of tube positions, cavity radius, and power input.

### 6.6.1 Evaluation of effects

Table 6.9 presents the main effects and binary interactions for receiver efficiency calculated from the fractional factorial design described in Table 6.8 with factors ordered from high to low effect magnitude at the lower of the two solar power ranges. Recall that low/high factor levels for  $Q_s$  are reversed in the 7-8 kW calculations.

	Effect (6 / 7 kW)	Effect (8 / 7 kW)		Effect (6 / 7 kW)	Effect (8 / 7 kW)
r <sub>cav</sub>	-1.79%	-1.74%	AD	-0.67%	-0.80%
$A/A_{max}$	-1.77%	-1.96%	$f_r$	0.66%	0.86%
$C_{feed}$	1.59%	2.28%	N <sub>max</sub>	-0.52%	-0.50%
$Q_s$	1.35%	-0.05%	AH	-0.48%	-0.30%
AG	1.08%	0.39%	AB	0.39%	0.19%
r/r <sub>max</sub>	-0.97%	-0.84%	AE	-0.12%	-0.13%
$f_2$	-0.92%	-0.96%	AC	0.003%	0.04%
AF	-0.89%	-0.94%			

Table 6.9: Effect magnitudes for Design 3 ( $2^{8-4}$  fractional factorial): reflective cavity

Parameters  $r_{cav}$ ,  $A/A_{max}$ , and  $C_{feed}$  have the strongest impact on receiver performance while the effect of  $f_r$  is less than half that of  $A/A_{max}$  regardless of solar power input. Thus while both factors position more carbon within the solar beam, it appears that removing the outer tubes and allowing energy to reflect off of the cavity walls is more effective than keeping the tubes in place to function as radiant absorbers. This implies that energy lost by conduction from radiant absorber tube ends exceeds that lost by absorption at cavity walls exposed by removal of the outermost tubes.

Solar power input has a large positive impact on efficiency in the range of 6-7 kW, but becomes negligible for 7-8 kW indicating approach to an optimum  $Q_s$  which is likely driven by the influence of increased emission losses at high power. The full alias structures (up to tertiary interactions) for the two most prominent binary interactions are AG+BC+DE+FH and AF+BE+CD+GH. The AG alias chain contains both the interaction between  $r/r_{max}$  and  $N_{max}$  and that between  $Q_s$  and  $C_{feed}$ . Each of these interactions was included among the significant effects in Designs 1 and 2 though the relative change in the magnitude of the interaction between 6-7 kW and 7-8 kW may imply that the interaction involving  $Q_s$  dominates. Though not shown in Table 6.9, the AG interaction exhibits negligible impact on receiver efficiency normalized by efficiency at complete carbon conversion providing further evidence for the dominance of the  $Q_s/C_{feed}$  interaction. The AF alias chain includes both the interaction between  $f_2$  and  $r/r_{max}$  as well as that between  $r_{cav}$  and  $Q_s$ , both of which were previously identified. Apart from  $Q_s$  and AG, the magnitudes of each main effect and binary interaction remain relatively unchanged for the two solar power ranges suggesting that optimal receiver configurations may be similar over a wide range of solar input.

#### 6.6.2 Relationship between responses

Relationships between receiver efficiency and  $\eta_1$ ,  $\eta_2$ ,  $X_{avg}$ , and  $X_{max}$  are similar to those shown in Figures 6.5-6.7 and 6.15-6.16 and the corresponding figures are not repeated here. Receiver efficiency can be nearly linearly correlated to  $\eta_1$  and  $X_{avg}$  with correlation coefficients of 0.95 for  $\eta_1$ , and 0.98 or 0.99 for  $X_{avg}$  with low or high carbon feed rate, respectively. Optimal efficiency again occurs at intermediate  $\eta_2$  with the best designs allowing energy to reflect off of the cavity wall. Figure 6.17 illustrates the relationship between receiver efficiency and fraction of energy lost by either emission or tube conduction for calculations with 6-7 kW solar power. Positive correlation (r = 0.62) occurs between efficiency and emission losses whereas negative correlation (r = -0.63) exists between efficiency and tube conduction losses. This corroborates the conclusion that keeping outer tubes in place to function at radiant absorbers, with the concomitant increase in tube conduction losses, is not an effective means of improving receiver performance. A third mechanism of energy loss occurs through reflection of solar energy or solar absorption by actively cooled surfaces and accounts for 15-34% of the solar input. A weak positive correlation (r = 0.35) occurs between efficiency and solar absorption/reflection losses.



Figure 6.17: Relationship between efficiency from Design 3 and the fraction of energy lost by (a) emission and (b) conduction along tube length

# 6.7 Design 4

Results from the previous three sections indicate that receiver configurations capable of achieving high efficiency typically contain three tubes clustered within the center of the receiver and pushed toward the back cavity wall. These designs are characterized by low  $A/A_{max}$  and  $N_{max}$ . All configurations with tubes residing outside the initial solar beam fail to achieve high conversion in the outermost tubes and suffer from large tube conduction losses. Thus tube configurations must be specified such that all tubes are placed in the solar beam; however, given parameter definitions detailed in Figures 6.1 and 6.2, only designs consisting of three tubes or

less are capable of meeting this specification. It remains to be seen if tube configurations consisting of more than three tubes placed within the solar beam offer any additional advantage. To this end a second method for specification of tube positions (method B) is detailed in Figure 6.3 and Appendix C. Figure 6.18 illustrates profiles of solar energy incident on the wall of an empty blackbody cavity at three distinct vertical coordinates and as a function of angle  $\beta$  with  $r_{cav} = 9.14$  cm (3.6 in). High solar incidence occurs in the region defined by  $\theta_c = 90^\circ$  over the entire cavity height. Solar energy incident on the cavity wall between  $\beta = 60^\circ$  and  $\beta = 130^\circ$  originates from the secondary angular bands visible in Figures 5.3 and 5.4.



Figure 6.18: Solar energy incident on the cavity wall with  $r_{cav} = 9.14$  cm in the absence of absorber tubes

Geometric receiver configurations based on the four factors specified in Table 6.10 are investigated in a 2<sup>4-1</sup> fractional factorial design consisting of eight simulations with constant  $r_{cav} = 9.14$  cm,  $Q_s = 7$  kW,  $C_{feed} = 6$  g/min, and  $\theta_c = 90^\circ$ . Efficiency ranges from 3.5% to 8.6% and the main effects are provided in Table 6.10. The number of tubes produces a strongly negative effect indicating that increasing the number of tubes does not improve receiver efficiency even when all tubes are contained within the solar beam. Furthermore, both factors  $r/r_{max}$  and  $f_2$  have relatively strong positive impacts indicating that, for this cavity size, tubes should remain along the back cavity wall with as large of a radius as possible. Binary interactions produce effects of 0.83%, -0.85%, and 0.51%, well under those calculated for three of the four main effects.

Factor	Name	Low level	High level	Effect
Α	r/r <sub>max</sub>	0.7	1	1.46%
В	$f_r$	1	2.5	0.72%
С	N	3	5	-2.48%
D	$f_2$	0.6	1	1.64%

Table 6.10: Factor levels and main effect magnitudes for Design 4 (2<sup>3-1</sup> fractional factorial): reflective cavity

## 6.8 Design 5

All results from previous sections point toward an optimal three-tube receiver configuration with tubes residing near the back cavity wall and within the central region of the cavity. Tables 6.2 and 6.9 indicate that increasing  $r_{cav}$  above 9.14 cm is detrimental, but values of  $r_{cav}$  below 9.14 cm have not yet been investigated. Figure 6.19 shows that the critical angle over which the largest quantity of direct solar energy is received is approximately independent of cavity radius between 6.6 and 9.14 cm. Cavity size, solar power, and carbon fed rate all strongly impact receiver performance, but optimal conditions cannot yet be ascertained as the previous studies do not assess response curvature. A central composite design (CCD) is utilized for this purpose and tube positions are specified using method B in Appendix C with constant  $\theta_c = 90^\circ$  and N = 3 regardless of cavity size.



Figure 6.19: Solar energy incident on the cavity wall in a horizontal plane aligned with the aperture centroid for  $r_{cav} = 9.14$  cm, 7.9 cm, and 6.6 cm in the absence of absorber tubes

Parameters  $f_2$  and  $r/r_{max}$  are important either as single factors or through binary interactions. Design 4 exclusively contains configurations approaching an optimal arrangement and indicates that, for  $r_{cav} = 9.14$  cm, the highest efficiency is achieved with  $f_2 = r/r_{max} = 1$  such that excessively small tube radii are prohibited. The optimal values of  $f_2$  and  $r/r_{max}$  are unlikely to decrease with cavity size and physical constraints prohibit increase of  $f_2$  and  $r/r_{max}$  above unity. Increasing the cross-sectional area of the center tube relative to that of the outer tubes produces a slight improvement in receiver efficiency, but an optimal  $f_r$  has yet to be determined. A fourfactor CCD based on a full 2<sup>4</sup> factorial design requires an identical number of calculations as a five-factor CCD based on a half-fraction of a  $2^5$  factorial. As the  $2^{5-1}$  fractional factorial is a resolution V design free from aliasing between main effects and binary interactions, there is little computational benefit to choosing the four-factor CCD assuming tertiary and higher interactions are insignificant. For this reason the parameter  $f_2$  is added into the CCD alongside  $r_{cav}$ ,  $Q_s$ ,  $C_{feed}$ , and  $f_r$  though previous results clearly suggest that optimal designs will set  $f_2$  equal to unity. A face-centered CCD is employed to avoid extreme values and because physical constraints prohibit  $f_2$  from exceeding unity. The resulting factor designations and low/high levels are summarized in Table 6.11. Ranges for  $f_2$ ,  $f_r$ ,  $Q_s$ , and  $C_{feed}$  are raised above those previously investigated as prior results indicate optimal performance at high levels. Specification of tube positions and operating conditions is completed by holding the remaining parameters constant at:  $\theta_c = 90^\circ$ , N = 3,  $f_1 = 0$ ,  $r/r_{max} = 1$ ,  $f_o = 0$ ,  $f_s = 0$ ,  $h_{cav} = 8$  in,  $R_{steam} = 1$ , and  $R_I = 0.5$  s<sup>-1</sup>.

Factor	Name	Low	High
1 40101	Ivanic	level	level
А	$f_2$	0.7	1
В	$f_r$	1.5	3
С	$r_{cav}$	2.6 in	3.6 in
D	$Q_s$	6.5 kW	7.5 kW
Е	$C_{feed}$	4 g/min	8 g/min

Table 6.11: Factor levels for Design 5 (five factor CCD): reflective cavity

The resulting receiver efficiency ranges from 6.9-13.1% with maximum temperature and reaction conversion varying between 1753-2209 K and 27-66% respectively. Notably the difference between the high and low maximum tube temperatures in any receiver configuration is less than 300 K, well below the 700 K observed for configurations studied in Design 1. Small cavity radius leads to absorbed solar flux as high as 2422 kW/m<sup>2</sup> and thus selection of an optimal design must include consideration of and, ideally, minimization of absorbed solar flux. Heat loss by tube conduction now accounts for only 17-35% of the total solar energy, whereas this value reached as high as 60% for unoptimized designs in Figure 6.9 and 6.17. Conversely, emission losses account for 33-42% of the total solar energy and are slightly higher than those observed for unoptimized designs in Figures 6.9 and 6.17.

A second order response surface model is fit to the predicted efficiency at treatment combinations dictated by the central composite design yielding an adjusted  $R^2$  value of 0.93. This simple model is capable of approximating efficiency at any CCD point within 0.5%.

Second order response surface models are also fit to the maximum absorbed solar flux and maximum tube temperature. Optima in the efficiency response are evaluated via the response surface model based on constraints imposed on the maximum absorbed solar flux shown in Table 6.12. The unconstrained optimum for this range of conditions produces a maximum efficiency of 13.2%, but the absorbed solar flux reaches nearly 1300 kW/m<sup>2</sup> with surface temperature exceeding 2000 K. Results in Table 6.12 indicate that the solar flux can be reduced to 1000 kW/m<sup>2</sup> while sacrificing less than 1% efficiency. Minimal variability in tube positions is noted for the configurations identified in Table 6.12. The selection of an optimum design capable of satisfying the solar flux constraint is largely driven by cavity size, solar power input, and feed conditions.

$\begin{array}{c} \operatorname{Max} q^{"}{}_{s,abs} \\ (\mathrm{kW/m}^2) \end{array}$	η	$T_{max}\left(\mathrm{K}\right)$	$f_2$	$f_r$	$r_{cav}$ (in)	$Q_s$ (kW)	C <sub>feed</sub> (g/min)
900	11.5%	1885	1	1.5	3.17	7.19	7.35
1000	12.3%	1921	1	1.5	3.07	7.47	7.56
1100	12.7%	1959	1	1.5	2.88	7.50	7.60
1200	13.0%	1992	1	1.5	2.73	7.50	7.60
1295	13.2%	2020	1	1.5	2.60	7.50	7.65

Table 6.12: Optimal design parameters and results for a reflective cavity

A representative set of contour plots generated from the response surface models for efficiency and absorbed solar flux are illustrated in Figure 6.20. All plots are generated in the vicinity of the optimum with the remaining three factors held constant at  $f_2 = 1$ ,  $f_r = 1.5$ ,  $r_{cav} = 3.07$  in,  $Q_s = 7.47$  kW, and  $C_{feed} = 7.56$  g/min. Maximum absorbed solar flux is controlled largely by the cavity radius. As expected, optimal designs retain high  $f_2$  with reductions in  $f_2$  increasing the maximum absorbed solar flux while failing to produce any improvement in receiver performance.



Figure 6.20: Contour plots from CCD response surface for (a) solar-to-chemical efficiency and (b) maximum absorbed solar flux (kW/m<sup>2</sup>)

Interactions between  $f_2$  and  $r_{cav}$  as well as  $Q_s$  and  $C_{feed}$  are plainly evident in Figure 6.20. Decreasing  $f_2$  has an adverse impact on receiver performance for any configuration, but this effect becomes comparatively more prominent at small cavity size. Similarly, receiver efficiency always increases with solar power under the conditions employed in Figure 6.20, but the impact of solar power is diminished when efficiency is restricted by low carbon feed rate. Maximum absorbed solar energy is primarily controlled by cavity radius and  $f_2$ , each of which dictates the proximity of the tube array to the focal point. Absorbed solar flux increases rapidly as the cavity radius decreases below 3 in, but decreases relatively slowly for a cavity radius above 3 in. As such, Table 6.12 shows that optimal designs for various solar flux constraints are clustered near a cavity radius of 3 in. All optimal designs maintain  $f_r$  at the lower boundary given by  $f_r = 1.5$ though Figure 6.20 indicates that variations in efficiency with  $f_r$  are extremely weak and thus a decrease in  $f_r$  below the lower limit is not likely to produce appreciable improvement in receiver performance.

### 6.9 Comparison of optimal and original designs

The optimal reflective cavity configuration is selected from Table 6.12 as that which produces a maximum absorbed solar flux of 1000 kW/m<sup>2</sup>. Calculation results from the combined Monte Carlo, finite volume and CFD models with  $C_{feed} = 7.56$  g/min and  $Q_s = 7.47$  kW are illustrated in Figure 6.21 and summarized in Table 6.13. Temperature profiles in Figure 6.21 exhibit a longer heated length and improved uniformity in tube temperature distributions compared to those for the existing configuration in Figure 5.18. Correspondingly, carbon conversion occurs throughout a larger tube region than that identified for the existing design in Figure 5.22.



Figure 6.21: (a) Profiles of temperature (K), (b) profiles of vertical velocity (m/s) in vertical and horizontal receiver slices, and (c) profiles of center tube carbon mass fraction for the optimal reflective cavity design

The response surface model predicts efficiency of 12.3%, maximum temperature of 1922 K, and maximum absorbed solar flux of 1000 kW/m<sup>2</sup>, all in close agreement with results from the detailed radiation and CFD model displayed in Table 6.13. Corresponding calculation results for the existing design under identical operating conditions are also shown in Table 6.13, though operation of the existing receiver under these conditions is physically unrealistic. The optimal design is predicted to achieve a solar-to-chemical efficiency nearly three times greater than that of the original design with this improvement predominantly originating from enhanced energy utilization within the tubes. The approximate net absorption efficiency ( $\eta_2$ ) is nearly 10% lower than that of the original design as more solar energy is allowed to strike the cavity wall. Yet the existing design utilizes only 10% of energy transferred into the tubes for the chemical reaction, while the corresponding value for the optimal design approaches 30%.

	Optimal	Original
η (%)	12.0	4.9
$X_{max}$ / $X_{avg}$ (%)	45 / 41	44 / 23
$\eta_1$ (%)	29.7	10.0
$\eta_2$ (%)	40.6	49.7
Max $q$ " <sub>s,abs</sub> (kW/m <sup>2</sup> )	1023	1520
Center tube $Q_{s,abs}/Q_s$ (%)	36.7	32.8
Outer tube $Q_{s,abs}/Q_s$ (%)	21.5	16.0 / 7.3
Center tube $T_{front}$ (K)	1929	1944
Center tube $T_{back}$ (K)	1629	1546
Outer tube $T_{max}$ (K)	1817	1631 / 1450
$N_{tubes}$	3	5
$r_{tube, center}$ (in) / $r_{tube, outer}$ (in)	0.49 / 0.40	0.50 / 0.50
Heat losses		
(% of solar input)		
Solar reflection	11.7	12.4
Solar absorption	7.5	7.3
IR transmission	12.0	8.4
IR absorption	23.8	14.6
Tube conduction	30.0	44.6
Cavity wall convection	4.2	7.2

Table 6.13: Comparison of optimal and original reflective cavity receiver designs with  $Q_s = 7.5$  kW and  $C_{feed} = 7.6$  g/min

Superior energy utilization in the tubes of the optimal design can be attributed to both a more uniform distribution of absorbed energy around the tube circumference as well as removal of tubes situated in regions which do not receive sufficient solar energy to attain high reaction conversion. Each outer tube in the optimal design absorbs more than 21% of the solar energy leading to maximum outer tube temperatures exceeding 1800 K. Outer tubes in the original design absorb at most 7-16% of the solar energy leading to maximum temperatures 170-350 K cooler than those predicted for the optimal design. As all tubes can be utilized for reaction, conductive heat loss from the tubes in the optimal design is responsible for only 30% of the solar

energy, compared to 45% in the original design. In accordance with Figures 6.9 and 6.17 emission losses are not minimized in the optimal design and account for 35% of the solar energy compared to 23% in the original design. The optimal design improves receiver performance while simultaneously reducing the maximum absorbed solar flux by nearly 500 kW/m<sup>2</sup> and lowering the front/back temperature discrepancy at the center tube by 100 K.

The center tube conversion for the optimal design is nearly indistinguishable from that for the original design despite a higher carbon feed rate and the concomitantly reduced residence time. Figure 6.22 illustrates profiles of the absorbed solar energy flux and temperature around the center tube circumference at three distinct vertical positions representing locations aligned with the aperture centroid (y = 0), the top of the aperture (y = 4.9 cm), and a point midway between the two (y = 2.5 cm).



Figure 6.22: Profiles of (a) absorbed solar flux and (b) temperature around the center tube circumference as a function of vertical position

The optimal design reduces the solar energy absorbed at the front of the tube while allowing a greater quantity of energy to reach the back of the tube thereby producing a more uniform temperature distribution around the surface. Furthermore, positioning the tube array in the back of the cavity increases the distance between the array and the focal point and allows the solar

beam to spread in the vertical dimension. This leads to increased solar absorption at the vertical extents of the aperture and results in both a longer heated tube length and diminished temperature gradients at the surface.

### 6.10 Evaluation of the optimal design at 1 MW

Industrially-scaled receivers can be expected to achieve higher efficiency than laboratoryscale designs due to low surface-to-volume ratios, particularly when convective and conductive losses are predominant. The impact of receiver scale on heat loss mechanisms and efficiency is assessed by scaling up the optimal configuration selected for 5-10 kW solar power to 1 MW. The window aspect ratio is kept identical to that in the existing laboratory-scale receiver and surface area is scaled proportionally to the solar power input. Solar flux as a function of dimensionless position at the window surface is assumed identical to that used in the models described above. All receiver dimensions are scaled in relation to the aperture size and flow rates are scaled in accordance with the solar input. The resulting tube radius is larger than the optimal laboratory-scale design by a factor of 11.6. Though flow is clearly laminar in the smallscale design with a Reynolds number less than 500, flow through the larger tubes is characterized by a Reynolds number between 2000-7000 depending on operating conditions. Computational fluid dynamics models for the large-scale receiver are carried out with a standard k- $\varepsilon$  closure model and the Reynolds averaged Navier-Stokes equations [25] in place of the simple laminar flow model used in the small scale design.

Table 6.14 provides calculations of receiver efficiency, reaction conversion, tube temperatures at the horizontal center plane, and heat losses for the design in Figure 6.21 at both 7.5 kW and 1 MW. Temperature profiles at the front and back surfaces of the center tube are

illustrated in Figure 6.23 as a function of the dimensionless vertical position with y/L = 0 defined at the top of the tube.

	7.5 kW	1 MW
η (%)	12.0	22.2
$X_{max}$ / $X_{avg}$ (%)	45 / 41	77 / 77
$\eta_1$ (%)	29.7	73.8
$\eta_2$ (%)	40.6	30.1
Center tube $T_{front}$ (K)	1929	1942
Center tube $T_{back}$ (K)	1629	1452
Outer tube $T_{max}$ (K)	1817	1856
Heat losses (% of solar input)		
Solar reflection	11.7	11.8
Solar absorption	7.5	7.6
IR transmission	12.0	15.1
IR absorption	23.8	30.3
Tube conduction	30.0	12.6
Cavity wall convection	4.2	4.9

Table 6.14: Performance of the optimal small-scale reflective cavity receiverconfiguration at 7.5 kW and 1 MW

The calculated receiver efficiency is 22%, though the linearly scaled flow rates from the small scale design may not be optimal at 1 MW. Maximum temperatures are analogous between designs with an increased center tube front / back temperature discrepancy at 1 MW arising from a comparatively larger tube radius. Tube conduction losses are substantially diminished at 1 MW as a result of a comparatively larger distance physically separating the hot zone from the top and bottom cooling zones. Emission losses by means of transmission or absorption by cooled cavity surfaces are correspondingly increased. Figure 6.23 indicates that the dimensionless heated tube length at 1 MW is substantially longer than that at 7.5 kW, and extends to just below or above the top and bottom cooling zones at y/L = 0.14 and 0.86

respectively. The longer heated length leads to higher conversion, improved utilization of energy transferred into the tubes (high  $\eta_1$ ), and higher efficiency, while the increased emission losses lead to lower absorption efficiency (low  $\eta_2$ ) compared to that predicted for the 7.5 kW receiver. The shift in the dominant mode of heat loss from conduction to emission implies that optimal designs at the laboratory scale may not necessarily be representative of optimal designs at an industrial scale. Characteristics of the large-scale receiver, namely long heated length, efficient energy utilization in the tube fluid, and minimal conductive losses, resemble those representative of absorbing cavity designs analyzed in the subsequent chapter. Optimization of the large-scale reflective design may more closely adhere to the principles discussed therein than those observed for a small-scale reflective cavity.



Figure 6.23: Center tube front and back temperature as a function of dimensionless vertical position for 7.5 kW and 1MW

# 6.11 Conclusions

The effects of fifteen distinct parameters describing receiver geometry, cavity size, and operating conditions on solar-to-chemical receiver efficiency were examined by means of a series of fractional factorial and central composite design studies. Geometric parameters were defined relative to a base design in which all tubes were arranged in a semicircle around the back cavity wall, and allowed for variations in the number, radius, and spatial arrangement of tubes. All designs were assessed for steam gasification of acetylene black via the computational model coupling heat, mass, momentum, chemical reaction, and radiation phenomena detailed in Chapter 5. Optimal designs were selected on the basis of the solar flux profile generated by the High Flux Solar Furnace at the National Renewable Energy Laboratory with solar power restricted to 8 kW. Variability in efficiency between individual receiver designs was dominated by cavity radius, solar power, and carbon feed rate.

Tubes positioned outside of the solar beam failed to reach temperatures high enough to carry out the gasification reaction and instead functioned as heat sinks conducting energy away from the hot zone and toward upper and lower cooling zones. Calculations indicated that conduction losses dominated over emission losses and thus maximizing the net absorption efficiency alone was not an effective means of improving receiver performance. Ideal configurations allowed a fraction of the solar energy to strike and reflect off of the cavity wall despite associated absorption losses. The reflected energy was preferentially directed toward the back side of the tube array and enhanced uniformity in distributions of absorbed solar energy and temperature around each tube surface. Thus providing energy to the tubes in manner conducive to energy utilization was more crucial than maximizing the net quantity of energy supplied.

Geometric receiver configurations yielding high efficiency typically contained three tubes clustered within the center of the receiver and situated near the back cavity wall. An optimal intermediate tube radius arose from competing effects pertaining to temperature uniformity and fluid velocity or residence time. In the limit of zero fluid velocity, radiative exchange between tube walls and entrained carbon particles dictates that the centerline temperature reaches, at best, a value intermediate to that attained at the front and back walls. Designs with small tubes allowed more solar energy to reflect off of the cavity wall than analogous designs with large tubes, and were characterized by a comparatively more uniform front/back temperature distribution and a correspondingly high centerline temperature in the zero-flow limit. However rapid centerline gas velocity resulting from the laminar flow profile and small tube radius impeded the approach of the actual centerline temperature to this limiting value. The centerline temperature in designs with large tubes more closely approached the theoretical zero-flow limit owing to comparatively slow gas velocity, but the limiting value was restricted by a low back wall temperature. Heat transfer within the tubes was predominantly governed by radiative exchange and the mean radiation penetration distance exceeded the tube radius for all designs indicating that, unlike convective and conductive transport, radiative transfer to the centerline was not hindered by a large tube size.

The unconstrained optimum solar-to-chemical efficiency determined from calculations in this study was 13.2%. A more physically realistic receiver design constrained the maximum absorbed solar flux to at most 1000 kW/m<sup>2</sup> and retained an efficiency of up to 12.3%, more than twice that of the original receiver configuration under identical operating conditions. The solar flux constraint was primarily enforced by cavity radius with minimal variability in spatial tube configurations noted between constrained and unconstrained designs. The optimal design was characterized by lower net absorption efficiency than the original design, but the absorbed energy was utilized more effectively within the tubes leading to conduction losses of only 30% of the solar input, compared to 45% for the original design. The optimal small-scale design was scaled linearly to accept 1 MW solar power and the predicted efficiency for the large-scale design exceeded 22% despite potentially unoptimized feed rates. The large-scale design was
characterized by comparatively low conduction losses, high emission losses, and superior utilization of absorbed energy. A shift in the dominant mode of heat loss from conduction to emission implied that optimal designs at the laboratory scale may not necessarily be representative of those at an industrial scale.

# Nomenclature

A	total tube surface area per unit length
$C_{feed}$	total carbon feed rate
$C_p$	molar heat capacity
$d_t$	distance between tube walls
$d_w$	minimum distance between cavity and tube walls
$f_l$	parameter describing offset of the back of the tube array toward the window
$f_2$	parameter describing tube semicircle radius
$f_o$	parameter describing offset of entire tube array toward window
<i>f</i> <sub>r</sub>	ratio of center tube cross-sectional area to outer tube cross-sectional area
$f_s$	parameter describing tube staggering
$h_{cav}$	cavity height
$l_m$	mean penetration distance for radiation
$\dot{n}_{C,o}$	inlet molar flow rate of carbon
N <sub>max</sub>	maximum number of tubes
$q"_{i,in}$	energy flux transferred into tube solid
$q''_{i,IR,abs}$	emitted energy flux absorbed by tube <i>i</i>
$q''_{i,IR,emitted}$	energy flux emitted by tube <i>i</i>
$q^{\prime\prime}_{i,solar,abs}$	solar energy flux absorbed by tube <i>i</i>
$Q_{reaction}$	energy used to carry out the endothermic reaction
$Q_s$	solar power (kW)
$Q_{tubes}$	energy transferred into the tube solid material
r	correlation coefficient

<i>r<sub>cav</sub></i>	cavity radius
r <sub>i</sub>	inner tube circle radius
r <sub>o</sub>	outer tube circle radius
$r_{o,max}$	maximum radius of outer tube semicircle
$r_t$	tube radius
$R_I$	standard inert gas flow rate / individual tube volume in front of window
R <sub>steam</sub>	molar ratio of steam to carbon feed rate
Т	temperature (K)
Х	fractional carbon conversion
η	solar-to-chemical receiver efficiency
$\eta_1$	ratio of energy used for reaction to energy transferred into tubes
$\eta_2$	ratio of energy transferred into tubes to solar energy input
$\eta_{abs.net}$	net absorption efficiency
$\eta_{max,C}$	receiver efficiency at 100% carbon conversion
$\eta_{max,rad}$	receiver efficiency if all solar energy not lost by emission of reflection is utilized
$ heta_c$	angular extent of tube array measured from cavity centroid
ρ	density
$ec{\upsilon}$	velocity
$\Delta H$	enthalpy of reaction

# References

- 1. Abanades, S., Charvin, P., and Flamant, G., Design and simulation of a solar chemical reactor for the thermal reduction of metal oxides: Case study of zinc oxide dissociation. *Chemical Engineering Science*, 2007. **62**(22): p. 6323-6333.
- 2. Lichty, P., Perkins, C., Woodruff, B., Bingham, C., and Weimer, A., Rapid High Temperature Solar Thermal Biomass Gasification in a Prototype Cavity Reactor. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(1).
- 3. Melchior, T., Perkins, C., Weimer, A.W., and Steinfeld, A., A cavity-receiver containing a tubular absorber for high-temperature thermochemical processing using concentrated solar energy. *International Journal of Thermal Sciences*, 2008. **47**(11): p. 1496-1503.

- 4. Palumbo, R., Keunecke, M., Moller, S., and Steinfeld, A., Reflections on the design of solar thermal chemical reactors: thoughts in transformation. *Energy*, 2004. **29**(5-6): p. 727-744.
- 5. Siegel, N.P., Ho, C.K., Khalsa, S.S., and Kolb, G.J., Development and Evaluation of a Prototype Solid Particle Receiver: On-Sun Testing and Model Validation. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(2).
- 6. Steinfeld, A. and Fletcher, E.A., A Solar Receiver-Reactor with Specularly Reflecting Walls for High-Temperature Thermoelectrochemical and Thermochemical Processes. *Energy*, 1988. **13**(4): p. 301-311.
- 7. Wieckert, C., Palumbo, R., and Frommherz, U., A two-cavity reactor for solar chemical processes: heat transfer model and application to carbothermic reduction of ZnO. *Energy*, 2004. **29**(5-6): p. 771-787.
- 8. Z'Graggen, A. and Steinfeld, A., Hydrogen production by steam-gasification of carbonaceous materials using concentrated solar energy V. Reactor modeling, optimization, and scale-up. *International Journal of Hydrogen Energy*, 2008. **33**(20): p. 5484-5492.
- 9. Dahl, J.K., Buechler, K.J., Weimer, A.W., Lewandowski, A., and Bingham, C., Solarthermal dissociation of methane in a fluid-wall aerosol flow reactor. *International Journal of Hydrogen Energy*, 2004. **29**(7): p. 725-736.
- 10. Hirsch, D. and Steinfeld, A., Radiative transfer in a solar chemical reactor for the coproduction of hydrogen and carbon by thermal decomposition of methane. *Chemical Engineering Science*, 2004. **59**(24): p. 5771-5778.
- 11. Meier, A., Bonaldi, E., Cella, G.M., Lipinski, W., Wuillemin, D., and Palumbo, R., Design and experimental investigation of a horizontal rotary reactor for the solar thermal production of lime. *Energy*, 2004. **29**(5-6): p. 811-821.
- 12. Melchior, T., Perkins, C., Lichty, P., Weimer, A.W., and Steinfeld, A., Solar-driven biochar gasification in a particle-flow reactor. *Chemical Engineering and Processing*, 2009. **48**(8): p. 1279-1287.
- 13. Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., Hydrogen production from solar thermal dissociation of natural gas: development of a 10 kW solar chemical reactor prototype. *Solar Energy*, 2009. **83**(9): p. 1599-1610.
- 14. Schaffner, B., Meier, A., Wuillemin, D., Hoffelner, W., and Steinfeld, A., Recycling of hazardous solid waste material using high-temperature solar process heat. 2. Reactor design and experimentation. *Environmental Science & Technology*, 2003. **37**(1): p. 165-170.

- 15. Schunk, L.O., Lipinski, W., and Steinfeld, A., Heat transfer model of a solar receiverreactor for the thermal dissociation of ZnO-Experimental validation at 10 kW and scaleup to 1 MW. *Chemical Engineering Journal*, 2009. **150**(2-3): p. 502-508.
- Steinfeld, A. and Spiewak, I., Economic evaluation of the solar thermal CO-production of zinc and synthesis gas. *Energy Conversion and Management*, 1998. **39**(15): p. 1513-1518.
- 17. Maag, G., Rodat, S., Flamant, G., and Steinfeld, A., Heat transfer model and scale-up of an entrained-flow solar reactor for the thermal decomposition of methane. *International Journal of Hydrogen Energy*, 2010. **35**(24): p. 13232-13241.
- Maag, G. and Steinfeld, A., Design of a 10 MW Particle-Flow Reactor for Syngas Production by Steam-Gasification of Carbonaceous Feedstock Using Concentrated Solar Energy. *Energy & Fuels*, 2010. 24: p. 6540-6547.
- 19. Tescari, S., Mazet, N., and Neveu, P., Constructal method to optimize solar thermochemical reactor design. *Solar Energy*, 2010. **84**(9): p. 1555-1566.
- 20. Tescari, S., Mazet, N., Neveu, P., and Abanades, S., Optimization Model for Solar Thermochemical Reactor: Efficiency Increase by a Nonuniform Heat Sink Distribution. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2011. **133**(3).
- 21. Melchior, T. and Steinfeld, A., Radiative transfer within a cylindrical cavity with diffusely/specularly reflecting inner walls containing an array of tubular absorbers. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2008. **130**(2).
- Haussener, S., Hirsch, D., Perkins, C., Weimer, A., Lewandowski, A., and Steinfeld, A., Modeling of a Multitube High-Temperature Solar Thermochemical Reactor for Hydrogen Production. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2009. 131(2).
- 23. Montgomery, D., *Design and Analysis of Experiments*. 6th ed. 2005, New York: John Wiley and Sons.
- 24. Trommer, D., *Thermodynamic and Kinetic Analyses of the Solar Thermal Gasification of Petroleum Coke*. 2006, Swiss Federal Institute of Technology: Zurich.
- 25. Versteeg, H.K. and Malalasekera, W., *An Introduction to Computational Fluid Dynamics*. 2<sup>nd</sup> ed. 2007, Harlow, England: Pearson Education.

# **Chapter VII**

# Optimization studies for a multiple tube solar receiver based on combined radiation and computational fluid dynamics modeling: Absorbing cavity

#### 7.1 Abstract

A three-dimensional, steady state computational model coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics for steam gasification of acetylene black is utilized to investigate the impact of parameters describing operating conditions and tube configurations on the solar-to-chemical efficiency of a multiple tube solar receiver with insulated absorbing cavity walls. Geometric factors are defined relative to a base design in which all tubes are arranged in a semicircle around the back cavity wall and allow for variations in cavity size, and number, radius, and arrangement of tubes with both staggered and nonstaggered arrangements considered along with factors allowing for offset of all or part of the tube semicircle toward the aperture. Tubes enclosed within an insulated absorbing cavity reach higher temperature than those within a cooled reflective cavity, with longer heated tube length and enhanced uniformity in temperature distributions arising from absorption of radiative energy emitted by the heated cavity wall. The ensuing reaction conversion and solar-to-chemical efficiency is correspondingly higher than that predicted for reflective cavity designs. Calculations indicate that maximizing net absorption efficiency and tube residence time while simultaneously minimizing solar energy incident on the cavity wall are critical to enhancing receiver performance. As such, ideal tube configurations are characterized by the maximum physically allowable tube size. Unlike reflective cavity designs, positioning tubes outside of the initial solar beam only detrimentally impacts receiver performance at excessively large cavity

size. Optimal designs typically contain three or five tubes arranged in a semicircle at the back cavity wall and calculations predict up to 35% solar-to-chemical receiver efficiency with temperature constrained at or below 1900 K. Enhanced efficiency over the tube configuration in the existing design is attributed to comparatively higher net absorption efficiency and increased residence time.

## 7.2 Introduction

The vast majority of receiver concepts proposed in the literature for high temperature solar-thermal processes include a heavily insulated refractory cavity wall [1-6], while cooled reflective cavity walls are encountered less frequently [7, 8]. Reflective cavity receivers are characterized by minimal thermal mass and are thus ideal for non-continuous experimental operation. However, utilization of a reflective boundary necessitates active cooling of outer surfaces as surface reflectivity of typical materials cannot be preserved in high temperature oxidizing environments. Furthermore, uncontrollable environmental variables produce an inherently transient solar input even during daylight hours. Absorber tubes cool rapidly in response to disruptions in solar power arising from passing clouds and thus tube materials are frequently and unavoidably exposed to thermal shock. Though the comparatively larger thermal mass and diminished surface area to volume ratio present at a large scale may marginally improve this behavior, reflective cavity receivers are likely infeasible for continuous operation at an industrial scale. The receiver cavity may alternatively be constructed of a refractory material and surrounded with an extensive insulation layer, thereby allowing heating of the cavity wall along with associated thermal emission. The considerable thermal mass theoretically allows for superior maintenance of internal receiver temperatures in response to transient interruptions in the power input [9-12]. Receiver efficiency for absorbing cavity designs scaled to accept up to

10 kW solar power typically ranges from 1-10% with heat losses primarily arising from emission (30-55% of  $Q_{solar}$ ) and conduction (30-65% of  $Q_{solar}$ ) [6, 9, 13-18]. Conductive losses are frequently attributable to active cooling of the quartz window, despite the heavily insulated cavity wall.

Only a limited number of studies detailed in the literature explore geometry optimization at a fixed scale [19-22], and these studies are commonly based on simplified receiver models which may not accurately depict all relevant physical and chemical processes. In the current study optimization calculations are carried out via a three-dimensional, steady state computational model coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics for steam gasification of acetylene black. The model described in Chapter 5 is modified to be valid for an absorbing insulated cavity and used to provide a physically realistic depiction of transport processes, temperature distributions, and chemical reaction kinetics. Sets of parameters describing receiver geometry and operating conditions are investigated by means of a series of fractional factorial and central composite design studies [23]. Fractional factorial designs are chosen to be, at minimum, resolution IV implying that main effects are aliased solely with tertiary interactions or higher [23]. All tube configurations originate from a base design with tubes arranged in a semicircle around the back cavity wall, and parameters describing receiver geometry and operating conditions are defined identically to those employed in the reflective cavity optimization studies in Chapter 6. Detailed calculations governing tube positions are described in Appendix C.

## 7.3 Receiver model

The experimentally validated computational model for heat, mass, momentum, chemical reaction, and radiation phenomena occurring in a reflective cavity receiver is detailed in Chapter

5 and summarized in Chapter 6. Calculations in this study are restricted to reactor configurations receiving at most 8 kW of solar energy with an aperture size identical to that of the existing reflective cavity receiver depicted schematically in Figure 1.1. The flux profile at the quartz window surface is that produced by the High Flux Solar Furnace (HFSF) at the National Renewable Energy Laboratory (NREL) as detailed in Chapter 5. All calculations are carried out with the ray directions and flux profile shape generated assuming an attenuator opening of 50%, and flux values are scaled linearly to yield the desired total power. Given the elevated temperatures necessary to achieve sufficient reaction conversion, the preferred tube material is silicon carbide. All calculations in this study are carried out with spatial mesh elements sized similarly to those producing a grid-independent solution for the existing receiver configuration in Chapter 5. Finite solid angle extents are specified as described in Chapters 4 and 5 by  $N_{\theta} = N_{\varphi} = 7$ .

Extension of the reflective cavity model described in Chapter 5 to an insulated absorbing cavity configuration is accomplished via modification of cavity wall boundary conditions. Specularly reflective polished aluminum cavity walls are replaced with diffuse-gray surfaces having a uniform absorptivity and emissivity of 0.85, with remaining material properties taken to be those of zirconia. Boundary conditions at the external cavity and tube walls are, for simplicity, derived from one-dimensional axial or radial conduction through the insulating layer. Heat flux conducted away from the external wall is described by equation 7.1 or 7.2 for, respectively, a cylindrical or planar surface where  $T_{ext}$  is the temperature of the external insulation surface,  $T_w$  is the wall temperature, and  $L_{ins}$  is the thickness of the insulation.

$$q_{w}^{"} = \frac{k(T_{w} - T_{ext})}{r \ln\left(1 + \frac{L_{ins}}{r}\right)}$$
(7.1)

$$q_{w}^{"} = \frac{k(T_{w} - T_{ext})}{L_{ins}}$$
 (7.2)

275

The external insulation temperature is held constant at 300 K and insulation thickness is assumed to be 13 cm (~5 in) or 5 cm (~2 in) for cavity and tube walls, respectively, with a constant thermal conductivity of 0.25 W/m/K. Calculations in this study are undertaken assuming a windowed aperture with active cooling around the quartz surface employed to maintain a constant 300 K external temperature. If tube and cavity materials are capable of withstanding high temperature oxidizing environments, then the indirectly irradiated multiple-tube receiver may be operated with an open aperture thereby eliminating the active cooling requirement and associated conductive losses.

Receiver configurations are evaluated for steam gasification of 42 nm carbon particles. Gasification kinetic parameters from Trommer et al. [24] produced superior predictions of experimental data and are used throughout this study. Solar-to-chemical efficiency of the multiple tube receiver was defined in equation 6.1 as the fraction of the incident solar power used to carry out the chemical reaction including sensible enthalpy requirements for the reactive components. Sensible enthalpy requirements for inert components or unconverted reactants are neglected.

#### 7.3.1 Reflective vs. absorbing cavity model results

The insulated, absorbing cavity wall reaches temperatures higher than those permitted by a reflective surface and, through thermal emission from the heated wall, produces a longer heated tube length, improved uniformity in tube temperature distributions and, correspondingly, higher average reaction conversion than observed with a reflective cavity boundary. Table 7.1 provides the solar-to-chemical receiver efficiency, maximum temperature and conversion in each tube, absorbed solar energy, net absorbed energy, and front/back temperature discrepancy for the center tube in the existing design with 7 kW solar power and a carbon feed rate of 1.2 g/min per tube. All operating conditions and simulation parameters are identical to those utilized in the sensitivity analysis in Chapter 5.8 with a reflective cavity. Figure 7.1 displays temperature profiles and carbon mass fraction in the center tube calculated from the computational fluid dynamics model with either an absorbing or reflective cavity wall.

	Reflective	Absorbing
η (%)	3.6	19.6
$\eta_1$ (%)	7	75
$\eta_2$ (%)	49	26
Center tube $\Delta T(K)$	380	246
<u>Center tube / Front tube /</u> <u>Back tube :</u>		
$T_{max}\left(\mathbf{K}\right)$	1874 / 1413 / 1591	2066 / 1778 / 1907
X (%)	40 / 5 / 13	79 / 71 / 75
$Q_{abs,\ solar}$ (kW)	2.3 / 0.51 / 1.1	2.2 / 0.41 / 1.0
$Q_{abs, net}$ (kW)	0.96 / 0.74 / 0.79	0.39 / 0.36 / 0.37
<u>Heat losses</u> (% of solar input) :		
Solar reflection	12.4	10.3
Transmission at window	8.4	29.4
Net absorption at cavity wall	22.0	30.4
Tube conduction	45.5	5.2

 Table 7.1: Comparison of calculations with a cooled reflective or insulated absorbing cavity wall for the existing receiver configuration

Tubes enclosed within an insulated absorbing cavity reach higher temperature than those within a cooled reflective cavity, with the temperature of the outer tubes increasing comparatively more than that of the center tube. While the center tube maximum temperature increases by less than 200 K from reflective to absorbing cavity designs, the front and back tube temperatures increase by, respectively, 365 K and 306 K. Coupled with an extended heated tube length, these elevated temperatures produce nearly uniform carbon conversion and feedstock utilization in the outer tubes thereby yielding a more than a threefold increase in receiver efficiency for the absorbing cavity design.



Figure 7.1: Profiles of temperature (K) for both (a) absorbing cavity and (b) reflective cavity and profiles of center tube carbon mass fraction for (c) absorbing cavity and (d) reflective cavity

Figure 7.1 reveals that the gasification reaction commences near the top of the center tube in the absorbing cavity design whereas reactants flow through nearly half of the tube length in the reflective cavity design before the reaction begins. This is a direct consequence of the lengthened heated region illustrated in detail in Figure 7.2. Figure 7.2 provides center tube surface temperature profiles as a function of angle  $\beta$  measured around the tube circumference within horizontal planes aligned with the center of the aperture (y = 0), the top of the aperture

(y = 5 cm), and approximately midway between the top of the aperture and the top of the cavity (y = 10 cm). The temperature at y = 10 cm and  $\beta = 0$  in the absorbing cavity model is more than 750 K hotter than that predicted from the reflective cavity model. Residence time in the hot zone is thus correspondingly longer for absorbing cavity designs and, as such, a larger carbon feed rate is permissible. The efficiency of the absorbing cavity design improves to 29% with 18 g/min carbon while a similar modification in carbon feed rate fails to improve performance of the reflective cavity design because residence time in the hot zone becomes inadequate.



Figure 7.2: Profiles of temperature around the center tube circumference for absorbing and reflective cavity configurations

Dominant heat loss mechanisms shift from conduction in reflective cavity designs to emission in absorbing cavity designs. Heat losses arising from conduction along the length of the tubes comprise 45% of the solar input in reflective cavity designs but only 5% in absorbing cavity designs on account of the insulated upper and lower cavity walls. Conversely, losses by transmission and net absorption at the cavity wall account for nearly 60% of the solar input in absorbing cavity designs, but only 30% in reflective cavity designs. Calculations for the existing reflective cavity receiver provided in Chapter 5 indicate that 90-95% of solar energy absorption

at the tube surfaces occurs prior to reflection. Thus the total quantity of solar energy absorbed by the tubular array when the cavity wall is strongly absorptive is only marginally lower than that when the cavity wall is reflective. Yet absorption of energy emitted by the insulated cavity wall produces a comparatively more uniform distribution of net absorbed energy. Net radiative energy absorption at the center tube is nearly 30% higher than that at the front tube in the reflective cavity design, but only 8% higher in the absorbing cavity design. Net radiative energy absorption by any tube for the absorbing cavity design is at best 50% that predicted for the reflective cavity design owing to the predominance of emission losses over conduction. Tubes contained within the cooled reflective cavity absorb more energy, but subsequently conduct a large fraction of this energy into the cooling zones.

Efficiency can be broken into two components as shown in Chapter 6 and equation 7.3: the ratio of energy used for reaction to the energy transferred into the tubes ( $\eta_1$ ), and the ratio of the energy transferred into the tubes to the total solar energy ( $\eta_2$ ).

$$\eta = \eta_1 \eta_2 = \frac{Q_{reaction}}{Q_{tubes}} \frac{Q_{tubes}}{Q_{solar}}$$
(7.3)

Table 7.1 and results in Chapter 6 reveal that reflective cavity receiver designs are characterized by poor utilization of absorbed energy and, as such, increasing  $\eta_I$  is critical to improving receiver performance. Conversely, Table 7.1 indicates that 75% of the energy transferred into the tubes in the absorbing cavity design is utilized to carry out the endothermic chemical reaction, yet only 26% of the solar input is transferred into the tubes. These observations suggest that, contrary to the results in Chapter 6, enhancing performance of absorbing cavity configurations may be closely tied to maximizing absorption efficiency.

# 7.4 Design 1

A resolution IV  $2^{13-8}$  fractional factorial design consisting of 32 simulations is exploited to investigate the four operating conditions and nine of the geometric parameters described in Figure 6.1. Tube positions are specified via method A and the factor  $f_r$  is omitted in the current design leading to tube arrays composed of uniformly-sized cylinders. Low and high factor levels are specified in Table 7.2. Design generators are F = ACE, G = BCE, H = ABC, J = CDE, K = ABCDE, L = ABE, M = ACD, and N = ADE. Main effects in the resulting design are aliased with tertiary interactions or higher whereas each binary interaction is aliased with four or five additional binary interactions. The resulting 32 receiver configurations and simulation results are provided in detail in Appendix D.

Factor	Name	Low	High
racioi	Inallie	level	level
А	$N_{max}$	5	9
В	$A/A_{max}$	0.6	1
С	$f_I$	0	0.4
D	$r/r_{max}$	0.6	1
Е	$f_2$	0.6	1
F	$f_o$	0	0.15
G	$f_s$	0	0.25
Н	$r_{cav}$	3.6 in	6 in
J	$h_{cav}$	8 in	14 in
Κ	$C_{feed}$	2 g/min	6 g/min
L	R <sub>steam</sub>	1	2
М	$R_I$	$1  \mathrm{s}^{-1}$	$2 \text{ s}^{-1}$
Ν	$Q_s$	4.8 kW	7.0 kW

 Table 7.2: Factor levels for Design 1 (2<sup>13-8</sup> fractional factorial):

 absorbing cavity

Calculated solar-to-chemical efficiency is provided in detail in Table D.7 in Appendix D and ranges from 0.2-19.4%, well above the maximum 6.4% achieved from an identical set of

reflective cavity configurations in Chapter 6. As discussed in Chapter 6, maximum achievable efficiency is restricted by both emission losses and carbon feed rate. Table D.7 reveals that the maximum efficiency based on emission and reflection losses ranges from 48-80% and is plainly less restrictive than the maximum efficiency based on complete carbon conversion which reaches at best 38%. The ratio of the efficiency to the maximal efficiency at complete carbon conversion reaches values as high as 92% suggesting that the range of carbon feed rates considered here may be substantially below optimal. The difference between the highest ( $T_{max}$ ) and lowest ( $T_{min}$ ) tube temperatures in a given configuration provides a metric by which temperature uniformity between tubes can be assessed. This difference ranges from 50-330 K for the factor levels in Table 7.2 and is substantially below the 110-690 K range observed for analogous reflective cavity designs in Chapter 6. The predominance of emission losses produces a low 9-50% range for net absorption efficiency compared to 20-78% for analogous reflective cavity designs.

#### 7.4.1 Evaluation of effects

Table 7.3 provides the main effects and binary interactions calculated from the fractional factorial design described in Table 7.2 for both  $\eta$  and  $\eta/\eta_{max,C}$ . Binary interactions are identified based on the factor designation for the first of five or six binary interactions present in a given alias chain. Factors are ordered from highest to lowest effect magnitude for receiver efficiency. Similar to reflective cavity configurations, variability in solar-to-chemical efficiency between designs is clearly dominated by carbon feed rate, cavity radius, and solar power input as designs with large  $r_{cav}$  or low  $Q_s$  fail to attain sufficiently high temperatures to carry out the gasification reaction and designs with low  $C_{feed}$  place an undesirably stringent restriction on maximum achievable efficiency. The impact of  $C_{feed}$  is greater than that observed in Chapter 6 as the average conversion is comparatively higher and, in certain cases, approaches 100%. The value

of  $\eta/\eta_{max,C}$  is approximately equivalent to the average conversion attained in the receiver and decreases strongly with carbon feed rate due to diminished residence time arising from the requisite increase in steam flow necessary to maintain a stoichiometric steam to carbon ratio. The negative effect of inert gas flow rate on receiver efficiency can similarly be attributed to residence time. High carbon feed rates may also potentially produce shading and blocking effects which inhibit radiative heat transfer to the tube centerline.

Effect		Effect		Effect		ect		
	η	$\eta/\eta_{max,C}$		η	$\eta/\eta_{max,C}$		η	$\eta/\eta_{max,C}$
$C_{feed}$	5.79%	-18.66%	$f_2$	-1.02%	-1.46%	AB	0.32%	1.90%
$Q_s$	4.34%	33.24%	AC	-0.98%	-5.17%	$N_{max}$	-0.28%	-2.01%
AH	3.30%	4.5%	AE	0.97%	4.43%	AJ	-0.28%	0.82%
r <sub>cav</sub>	-2.86%	-10.87%	$A/A_{max}$	-0.97%	-4.59%	AF	0.27%	0.01%
$R_I$	-2.79%	-12.69%	R <sub>steam</sub>	-0.94%	-0.95%	AK	-0.27%	-2.36%
AN	-1.95%	-4.19%	r/r <sub>max</sub>	-0.84%	-2.44%	BN	0.18%	0.54%
AL	-1.55%	-1.50%	BD	-0.75%	-4.55%	ABD	-0.18%	-2.23%
AM	-1.54%	-6.52%	AG	-0.50%	-0.87%	$f_s$	0.10%	-3.01%
AD	1.07%	6.19%	ABN	-0.41%	0.70%	$f_o$	-0.04%	0.98%
BM	-1.03%	-4.17%	ABM	0.39%	-0.64%	$h_{cav}$	0.01%	-1.54%
						$f_{I}$	0.00%	-0.32%

Table 7.3: Effect magnitudes for Design 1 (2<sup>13-8</sup> fractional factorial): absorbing cavity

As noted for Design 1 in Chapter 6, identification of significant geometric parameters is hindered by the large spread in receiver efficiency and the dominance of operating conditions and cavity size. The combination of low  $Q_s$  and high  $r_{cav}$  severely limits tube temperatures and these low temperatures, coupled with low  $C_{feed}$ , place considerable restriction on attainable receiver efficiency regardless of tube configuration. Nevertheless, the main effects of  $f_s$ ,  $f_o$ ,  $f_1$ , and  $h_{cav}$  are clearly negligible and the choice of the maximum number of tubes is of little consequence compared to that observed for reflective cavity designs. Factors  $f_s$ ,  $f_o$ , and  $f_l$  modify spatial positioning without introducing variations in size or number of tubes and the irrelevance of these factors implies that receiver performance is insensitive to tube positioning alone. The relative insignificance of cavity height suggests that little to no reaction conversion occurs outside of the lower cavity height limit despite heated upper and lower tube regions.

Various binary interactions appear among the parameters with the largest impact on efficiency in Table 7.3. The most significant, identified by their full alias structure up to tertiary interactions are: AH+BC+EG+FL+KN, AN+CJ+DE+FM+HK, AL+BE+CG+FH+KM and AM+CD+EJ+FN+KL. The convoluted alias structure present in the screening design prohibits identification of the exact nature of the interactions responsible for the observed effects. Yet given the relative magnitudes of the constitutive main effects it seems probable that the AHinteraction results from  $C_{feed}$  and  $Q_s$  (KN). This interaction implies that solar power has a stronger positive impact on efficiency at high carbon feed rates than low, and is attributable to the efficiency limitation at complete carbon conversion. The AH alias chain has minimal effect on  $\eta/\eta_{max,C}$  implying that modifications in  $Q_s$  produce analogous impacts on average carbon conversion at both low and high carbon feed rate. Excluding all interactions involving negligible main effects  $N_{max}$ ,  $f_1$ ,  $f_s$ ,  $f_o$ , or  $h_{cav}$ , the remaining binary interactions are most likely attributed to  $r/r_{max}$  and  $f_2$  (DE) or  $r_{cav}$  and  $C_{feed}$  (HK),  $C_{feed}$  and  $R_I$  (KM), and  $C_{feed}$  and  $R_{steam}$  (KL). Each interaction produces a comparatively larger impact on  $\eta$  than on  $\eta/\eta_{max,C}$  suggesting the involvement of C<sub>feed</sub>. Averages in the efficiency response at relevant treatment combinations indicate that cavity radius, steam to carbon ratio, and inert gas flow rate each have a larger negative effect at high than at low carbon feed rate, and the KM and KL interactions highlight the necessity of maintaining sufficient residence time with large feed rates.

#### 7.4.2 Relationship between responses

Equation 7.3 describes the breakdown of efficiency into two components: the ratio of the energy used for the reaction to the energy transferred into the tubes ( $\eta_1$ ), and the ratio of the energy transferred into the tubes to the total solar energy ( $\eta_2$ ). Figure 7.3 suggests that, contrary to trends observed for reflective cavity designs in Chapter 6, highly efficient absorbing cavity designs require maximization of both absorption efficiency and utilization of absorbed energy though a much stronger positive correlation exists between  $\eta$  and  $\eta_1$  (r = 0.76) than between  $\eta$  and  $\eta_2$  (r = 0.06).



Figure 7.3: Receiver efficiency from Design 1 as a function of (a)  $\eta_1$  and (b)  $\eta_2$ 

Figure 7.4 depicts no discernible trend relating receiver efficiency to the fraction of solar energy absorbed by the cavity wall surface and implies that allowing solar energy to reach the cavity wall is neither beneficial nor detrimental to receiver performance for these conditions. On the contrary, reflective cavity configurations clearly benefited from allowing solar energy to strike the cavity surface, typically within the region designated by  $\beta = 60-120^{\circ}$  in Figure 6.17. This solar energy was specularly reflected and preferentially directed toward the tube array thereby producing augmented solar incidence at the back of the array and enhanced uniformity in

temperature profiles. Solar energy reaching the absorbing cavity wall, on the other hand, is either diffusely reflected or absorbed and diffusely emitted, and the resultant loss of directional history for the radiative energy ensures that the reflected or emitted energy is not preferentially directed toward the tube array. As the directional history of the solar energy cannot be retained, it becomes inconsequential whether the cavity wall is heated by direct solar absorption or by absorption of energy emitted by heated surfaces.



Figure 7.4: Receiver efficiency from Design 1 as a function of cavity wall solar absorption efficiency

Under the conditions described by Table 7.2, efficiency increases nearly linearly with both average carbon conversion ( $X_{avg}$ ) and maximum carbon conversion ( $X_{max}$ ), with separate linear relationships observed for the two distinct carbon feed rates illustrated in Figure 7.5. The maximum and average carbon conversion differ on average by only 4.5% and, unlike reflective cavity configurations, improvements in maximum conversion are an equally effective means of enhancing receiver efficiency as those in average conversion. Uniformity in reaction conversion between tubes arises from the influence of cavity wall emission which reduces the sensitivity of receiver performance to tube positions. Thus while optimization of reflective cavity designs was

largely driven by improving the distribution of energy between tubes and removing tubes from regions with minimal solar energy, this does not appear to be directly relevant in absorbing cavity configurations.



Figure 7.5: Receiver efficiency from Design 1 as a function of (a) average and (b) maximum carbon conversion



(a) net cavity wall absorption and (b) transmission

The principle mechanism of energy loss is emission by the heated tube surfaces which occurs via both transmission through the transparent window, and net absorption at the cavity wall. Emission losses account for 38-75% of the total solar energy, whereas losses by tube conduction are responsible for only 2-10% of the solar input. Figure 7.6 relates receiver efficiency to emission losses by net absorption at the cavity surface and by transmission. Correlation coefficients describing these relationships are -0.35 and 0.19, respectively, indicating a slight preference for transmission losses over absorption.

#### **7.5 Design 2**

The results from Design 1 reveal that carbon feed rate, solar power, cavity radius and associated binary interactions play a strong role in controlling receiver efficiency. While tube positioning appears to be comparatively less important, evaluation of parameters describing receiver geometry is hindered by poor receiver performance observed at low  $Q_s$ , low  $C_{feed}$ , and high  $r_{cav}$ , regardless of tube configuration. As only receiver configurations capable of producing high efficiency are of interest, a subset of parameters describing receiver geometry are reevaluated under constant operating conditions. A resolution IV 2<sup>6-2</sup> fractional factorial design consisting of 16 simulations is utilized to investigate six parameters describing tube configurations with low and high factor levels specified in Table 7.4. Operating conditions and cavity size are held constant at values leading to superior performance:  $R_I = 0.5 \text{ s}^{-1}$ ,  $C_{feed} = 6 \text{ g/min}, R_{steam} = 1, Q_s = 7 \text{ kW}, r_{cav} = 9.14 \text{ cm} (3.6 \text{ in}), \text{ and } h_{cav} = 20.3 \text{ cm} (8 \text{ in}).$  Tube positions are specified via method A in Appendix C with  $f_o = f_1 = 0$  based on relatively negligible effect magnitudes observed in Design 1. Parameter  $f_r$  is introduced into the design to allow differentiation between center and outer tube radii. Design generators are E = ABC and F = BCD. Main effects in the resulting design are aliased with tertiary or higher interactions whereas each binary interaction is aliased with at most one other binary interaction [23]. The resulting 16 receiver configurations and simulation results are provided in detail in Appendix D. Factor designations are maintained equivalent to those in Design 1 wherever possible to

minimize pre-processing and computational requirements. Calculated solar-to-chemical efficiency ranges from 10.8-21.8% with maximum temperature and carbon conversion varying between 1967-2145 K and 44-84% respectively. The calculated efficiency approaches 39-78% of the maximum efficiency at complete carbon conversion.

Factor	Name	Low level	High level
А	$N_{max}$	5	9
В	$A/A_{max}$	0.6	1
С	$f_r$	1	2.5
D	r/r <sub>max</sub>	0.6	1
Е	$f_2$	0.6	1
F	$f_s$	0	0.25

Table 7.4: Geometric factor levels for Design 2 (2<sup>6-2</sup> fractional factorial): absorbing cavity

#### 7.5.1 Evaluation of effects

Table 7.5 presents the main effects and binary interactions for receiver efficiency calculated from the fractional factorial design described in Table 7.4 with factors ordered from high to low effect magnitude.

	Effect		Effect
r/r <sub>max</sub>	3.72%	$A/A_{max}$	0.78%
$f_2$	3.49%	AC + BE	-0.61%
N <sub>max</sub>	-2.43%	$f_r$	0.44%
AF + DE	-1.73%	AB + CE	0.15%
AE + BC	1.27%	BF + CD	-0.14%
AD + EF	1.00%	$f_s$	-0.04%
BD + CF	-0.79%		

Table 7.5: Effect magnitudes for Design 2 (2<sup>6-2</sup> fractional factorial): absorbing cavity

These effect magnitudes are notably different than those in Table 7.3 signifying non-negligible interactions between receiver geometry and operating conditions or cavity size. Effect magnitudes listed in Table 7.5 are evaluated exclusively at levels of operating conditions and cavity size producing superior receiver performance and are thus of greater relevance than those displayed in Table 7.3.

Variability in efficiency between configurations is dominated by main effects  $r/r_{max}$ ,  $f_2$ , and  $N_{max}$  with little influence from  $N/N_{max}$ ,  $f_r$ , or  $f_s$ . This behavior is consistent with that observed in Design 1 and further corroborates the conclusion that modifications in tube position alone are incapable of enhancing receiver performance. Tube radii modifications are accomplished via the comparatively more significant parameters  $r/r_{max}$ ,  $f_2$ , and  $N_{max}$ . Low levels of  $r/r_{max}$  and  $f_2$  lead to identical variations in tube radius with parameter  $f_2$  producing a simultaneous modification in tube position. The similarity in the  $r/r_{max}$  and  $f_2$  main effects suggests that the  $f_2$  effect results predominantly from tube radius rather than from positional modifications. The sizeable positive effect of each  $r/r_{max}$  and  $f_2$  designates an optimally large tube radius along with a correspondingly high absorber surface area and long residence time. Parameter  $N_{max}$  is defined such that total absorber surface area is kept constant, and thus the large negative effect produced by  $N_{max}$ highlights the importance of long residence time over that of high surface area. There is no clear advantage gained from preferentially placing the carbon feed within the initial solar beam by means of low  $A/A_{max}$  or high  $f_r$ . Removal of the outlying tubes leads to slightly higher average array temperature, but also reduced residence time as the same carbon feed flows though a proportionally smaller number of tubes. The positive  $A/A_{max}$  effect displayed in Table 7.5 signifies that, for absorbing cavity designs, maximizing residence time is of greater concern than maximizing average tube temperature under these conditions.

Based on the magnitude of constitutive main effects, the notable binary interactions most probably arise from  $r/r_{max}$  and  $f_2$  (*DE*),  $N_{max}$  and  $f_2$  (*AE*), and  $r/r_{max}$  and  $N_{max}$  (*AD*). Response averages at the relevant treatment combinations are displayed in Table 7.6. All three interactions involve tube radius with parameter  $r/r_{max}$  having a stronger positive effect at high  $N_{max}$  or low  $f_2$ , and parameter  $f_2$  having a larger positive effect at high  $N_{max}$ . Each interaction emphasizes the necessity of maintaining large tube radii.

 Table 7.6: Average efficiency at various treatment combinations from Design 2

D	Е (	$(f_2)$	А	Е (	$f_2$ )	А	D ( <i>r</i> /	$(r_{max})$
$(r/r_{max})$	Low	High	$(N_{max})$	Low	High	$(N_{max})$	Low	High
Low	14.0%	19.3%	Low	18.6%	20.8%	Low	18.4%	21.1%
High	19.5%	21.3%	High	14.9%	19.7%	High	14.9%	19.7%

Though the same subset of main effects and binary interactions impacts both absorbing and reflective cavity designs, the nature of these effects is altogether different. Binary interactions in the reflective cavity calculations designated an optimal intermediate tube radius whereas Figure 7.7 and Table 7.6 identify an ideal maximum tube radius for absorbing cavity designs.



Figure 7.7: Relationship between efficiency from Design 2 and (a) outer tube radius or (b) total absorber area per unit length

#### 7.5.2 Relationship between responses

Figure 7.8 shows that, at operating conditions which produce superior receiver performance, maximizing absorption efficiency  $(\eta_2)$  is essential for achieving high receiver efficiency. Reflective cavity results were characterized by poor utilization of absorbed energy and highly efficient designs allowed energy to strike the cavity wall at the expense of absorption efficiency in order to deliver solar energy to the tube array in a manner conducive to energy The longer heated length and relatively uniform inter-tube temperature profiles utilization. characteristic of absorbing cavity designs lead to utilization of greater than 65% of net absorbed energy, regardless of tube configuration. Conversely, net energy absorption by the tube array comprises at best 30% of the solar input and varies by nearly a factor of two with respect to tube configuration. Thus, contrary to reflective cavity results, improvements in receiver performance stem predominantly from an increase in absorption efficiency. Correspondingly, Figure 7.9 illustrates that allowing solar energy to strike the cavity wall is detrimental to receiver performance because the diffuse nature of the cavity surface eliminates the directional history of the solar beam such that reflected or re-emitted energy is not preferentially directed toward the tube array.



Figure 7.8: Receiver efficiency from Design 2 as a function of (a)  $\eta_1$  and (b)  $\eta_2$ 



Figure 7.9: Receiver efficiency from Design 2 as a function of cavity wall solar absorption efficiency

Optimally efficient absorbing cavity designs are those which are characterized by comparatively long residence time. The residence time provided in Figure 7.10 is the nominal plug flow residence time within the entire tube length at standard conditions in the absence of gas thermal expansion and is an overestimation of the realistic residence time.



Figure 7.10: Receiver efficiency from Design 2 as a function of nominal plug flow residence time at standard conditions

Designs with large tubes are characterized by both long residence time and high solar absorption efficiency. Thus the observed increase in efficiency with tube radius cannot be unambiguously

attributed to either characteristic; through the large negative effect of  $N_{max}$  at constant absorber area suggests that the residence time effect is dominant. Calculation results exhibit a nearly linear correlation between both average and maximum reaction conversion. This behavior is analogous to that observed in Figure 7.5 and the corresponding illustrations are not repeated.

## 7.6 Design 3

Results from the previous sections indicate that cavity size, solar power, and carbon feed rate all strongly impact receiver performance, but optimal conditions cannot yet be ascertained as the previous studies do not assess response curvature. A central composite design (CCD) is utilized for this purpose and two parameters in addition to those listed above are selected for inclusion in the design. Increases in either inert gas flow rate or the molar steam to carbon ratio decrease the carbon conversion and receiver efficiency by means of a shortened residence time.  $R_I$  is held constant at 0.25 s<sup>-1</sup> as there is no theoretical advantage to be gained by increasing inert gas flow rate above a physically realistic minimum value. Similarly high steam flow rate negatively impacts receiver efficiency by restricting residence time, but the steam to carbon molar ratio cannot be decreased below unity without placing a stoichiometric limit on carbon conversion. Given the high carbon conversion attained in the calculations, a constant molar steam to carbon ratio of 1.25 is chosen for the current study. Calculations from Design 2 under desirable operating conditions of high  $Q_s$  and  $C_{feed}$  with low  $r_{cav}$ ,  $R_I$ , and  $R_{steam}$  indicate that geometric parameters  $f_2$  and  $r/r_{max}$  have the largest impact on receiver performance and optimal configurations contain large tubes characterized by  $f_2 = r/r_{max} = 1$ . Physical restrictions prohibit additional increase in either  $f_2$  or  $r/r_{max}$  and, as such, both are held constant in the current design. Table 7.5 suggests an optimally small number of tubes, but this conclusion is based on a consideration of arrays containing up to nine tubes. The number of tubes is included as a variable in the central composite design to assess values intermediate to those considered in the fractional factorial designs. The remaining factors describing receiver geometry in Designs 1 and 2 had only minimal impact on receiver performance.

However, as discussed in Chapter 6, a four-factor CCD based on a full 2<sup>4</sup> factorial design requires an identical number of calculations as a five-factor CCD based on a half-fraction of a 2<sup>5</sup> factorial. As the  $2^{5-1}$  fractional factorial is a resolution V design free from aliasing between main effects and binary interactions, there is little computational benefit to choosing the four-factor CCD assuming tertiary and higher interactions are insignificant. For this reason parameter  $\theta_c$  is included as the fifth factor in the design and tube positions are specified via method B in Appendix C. A face-centered CCD is employed to both avoid extreme values and restrict the number of tubes to an integer value. Table 7.7 presents the factor designations alongside low and high bounding values. The upper limit of carbon feed rate is extended above that previously considered as efficiency calculated in Designs 1 and 2 approached 80% of the maximum value at complete carbon conversion. Insignificant factors are held constant at  $f_0 = 0$ ,  $f_s = 0$ ,  $f_r = 0$ ,  $f_l = 0$ , and  $h_{cav} = 20.3$  cm (8 in). Full results in Appendix D show that the maximum absorbed solar flux typically remains below the desired limit of 1100 kW/m<sup>2</sup> imposed in Chapter 6; however, the maximum temperature approached 2150 K for a cavity radius of 9.14 cm (3.6 in). Hexoloy SA silicon carbide tubes are typically installed in the existing receiver and are capable of continuous operation in air up to 1900°C (2143 K). Given the transient and unidirectional nature of the heating source, it is advantageous to restrict this maximum temperature to values substantially below the operating limit. Maximum temperature is closely connected with the proximity of the tube array to the focal point which, in turn, is controlled by the cavity radius.

Thus the minimal cavity radius is chosen to be 3.6 in despite calculations indicating improved efficiency with small cavity size.

Factor	Name	Low level	High level
А	N	3	7
В	$ heta_c$	120	180
С	$r_{cav}$	3.6 in	6 in
D	$Q_s$	6 kW	8 kW
Е	$C_{feed}$	8 g/min	24 g/min

Table 7.7: Factor levels for Design 3 (5 factor CCD): absorbing cavity

The resulting central composite design, receiver configurations and simulation results are provided in detail in Appendix D. Receiver efficiency ranges from 11-35% with maximum temperature and reaction conversion varying between 1531-1879 K and 12-75% respectively. Average conversion ranges from 11-70% and is only slightly lower than the calculated maximum conversion. Maximum temperatures are reduced below those calculated in Designs 1 and 2 owing to a larger heat sink for the endothermic reaction provided by high carbon feed rate.

A second order response surface model is fit to the predicted efficiency at treatment combinations dictated by the central composite design yielding an adjusted  $R^2$  value of 0.99. This simple model is capable of approximating efficiency at any CCD point within 0.9%. Second order response surface models are also fit to the maximum tube temperature and the front/back temperature discrepancy at the center tube surface. Optima in the efficiency response are evaluated via the response surface model based on constraints imposed on the maximum temperature shown in Table 7.8. The unconstrained optimum for this range of conditions produces a maximum efficiency of nearly 36%, with a maximum temperature exceeding 1950 K. Results in Table 7.8 indicate that the maximum temperature can be reduced to 1900 K while

sacrificing less than 0.5% efficiency. Maximum tube temperature is largely controlled by cavity radius, though restriction of temperature below 1800 K also utilizes a simultaneous increase in the number of tubes and decrease in  $\theta_c$ . Large tube radius generated by both high  $\theta_c$  and small N positions the front of the center tube close to the focal point and contributes to a high maximum temperature.

Max T (K)	η	N	$ heta_c$	r <sub>cav</sub>	$Q_s$ (kW)	$C_{feed}$ (g/min)
1600	25.9%	5	120	6	6.3	16.9
1700	32.1%	5	131	6	8.0	19.9
1800	34.4%	5	180	4.9	8.0	18.7
1900	35.4%	3	180	4.1	8.0	18.1
1960	35.9%	3	180	3.6	8.0	17.3

Table 7.8: Optimal design parameters and results for an absorbing cavity

A representative set of contour plots generated from the response surface model are illustrated in Figure 7.11 for both efficiency and maximum temperature. All plots are generated in the vicinity of the optimum with the remaining three factors held constant at N = 3,  $\theta_c = 180^\circ$ ,  $r_{cav} = 4.1$  in,  $Q_s = 8$  kW, and  $C_{feed} = 18.1$  g/min. Interactions between parameters  $Q_s$  and  $C_{feed}$ ,  $\theta_c$ and  $r_{cav}$ , and N and  $r_{cav}$  are readily apparent. Maximum temperature is altered relatively more by cavity radius than by solar power input and thus limitations on maximum temperature shown in Table 7.8 are principally imposed via cavity radius. Large carbon feed rate may also reduce maximum temperature owing to the comparatively higher endothermic reaction heat sink. Selection of carbon feed rate for optimal receiver performance requires balancing the short residence time with the high limiting efficiency at complete conversion produced by high feed rates.



Figure 7.11: Contour plots from the CCD response surface for (a) solar-to-chemical efficiency and (b) maximum temperature (K)

Figure 7.11 indicates that though three tubes are optimal with a small cavity radius, this value shifts to a comparatively larger number of tubes as the cavity radius increases. Selection of  $\theta_c$  results from balancing the desired maximum tube surface area and residence time produced by  $\theta_c = 180^\circ$  with the enhanced temperature uniformity produced by  $\theta_c = 120^\circ$ . Figure 7.11 suggests that the former effect dominates at low cavity radius whereas the latter dominates at high cavity radius when the outlying tubes are potentially situated far outside of the solar beam.

### 7.7 Comparison between optimal and original designs

The optimal absorbing cavity configuration is selected from Table 7.8 as that which produces a maximum temperature of 1900 K. Calculation results from the combined Monte Carlo, finite volume and CFD models with  $Q_s = 8$  kW and  $C_{feed} = 18.1$  g/min are illustrated in Figure 7.12 and summarized Table 7.9. Temperature profiles are reminiscent of those depicted in Figure 7.1 for the existing receiver design. Heated tube lengths are similarly sized while the fluid temperature in the optimal design is comparatively lower than the tube wall on account of higher flow rates. The response surface model predicts efficiency of 35.4% and maximum temperature of 1900 K, both in close agreement with results from the detailed radiation and CFD model displayed in Table 7.9. Corresponding calculation results for the existing receiver configuration under identical operating conditions are also shown in Table 7.9, though operation of the existing receiver under these conditions is physically unrealistic. Predicted solar-tochemical efficiency for the optimal configuration is only 7% higher than that for the original configuration. However, unlike the existing receiver configuration, the optimal design produces this efficiency without exceeding limits imposed on maximum surface temperature or absorbed solar flux.



Figure 7.12: (a) Profiles of temperature (K), (b) profiles of vertical velocity (m/s) in vertical and horizontal receiver slices, and (c) profiles of center tube carbon mass fraction for the optimal absorbing cavity design

	Optimal	Original
η (%)	36	29
$X_{max}$ / $X_{avg}$ (%)	61 / 51	57 / 45
$\eta_1$ (%)	70	67
$\eta_2$ (%)	51	44
Max $q''_{s,abs}$ (kW/m <sup>2</sup> )	948	1541
Center tube $T_{front}$ (K)	1920	2058
Center tube $T_{back}$ (K)	1470	1724
Outer tube $T_{max}$ (K)	1742	1680 / 1830
$N_{tubes}$	3	5
$r_{tube}$ (in)	1.1	0.5
Heat losses		
(% of solar input)		
Solar reflection	10.2	10.3
Transmission at window	15.7	19.0
Net absorption at cavity wall	20.1	23.5
Tube conduction	3.3	3.8

Table 7.9: Comparison of optimal and original absorbing cavity receiver designs with  $Q_s = 8$  kW and  $C_{feed} = 18.1$  g/min

Figure 7.13 illustrates profiles of the surface temperature and solar energy flux absorbed around the center tube circumference at three distinct vertical positions representing locations aligned with the aperture centroid (y = 0), the top of the aperture (y = 4.9 cm), and a point midway between the two (y = 2.5 cm).



Figure 7.13: Profiles of (a) absorbed solar flux and (b) temperature around the center tube circumference as a function of vertical position

The relatively longer distance physically separating the tube array from the focal point in the optimal configuration allows the solar beam to spread in the vertical dimension such that the optimal design is characterized by comparatively high solar incidence at the vertical extents of the aperture. However, cavity wall emission serves to balance out distributions of net absorbed energy such that the augmented solar incidence at y = 4.9 cm in the optimal design is not reflected in corresponding temperature profiles. The optimal design produces a center tube front/back temperature discrepancy nearly 120 K higher than that predicted for the original design, but the resultant temperature gradients occur across nearly double the tube radius. The optimal design is characterized by higher carbon conversion owing to longer residence time despite maximum temperatures lower than those predicted for the original tube configuration. Relative distributions between heat loss mechanisms remain essentially unchanged with the

optimal design exhibiting slightly lower transmission losses as a result of lower maximum tube temperatures and larger distance between the tube array and the aperture. The comparatively higher efficiency of the optimal design can be attributed to a larger absorption efficiency (51%) compared to that predicted for the original design (44%) while utilization of absorbed energy is nearly indistinguishable between the two designs.

#### 7.8 Evaluation of the optimal design at 1 MW

Industrially-scaled receivers can be expected to achieve comparatively higher efficiency than laboratory-scale designs due to small surface-to-volume ratios. Calculations in Chapter 6 indicated that an optimized reflective cavity receiver with 12% efficiency at 8 kW could be theoretically expected to reach at least 22% at 1 MW. However, the size scale may not be as beneficial for absorbing cavity designs because emission losses dominate over convective and conductive losses. In order to assess the impact of receiver size on efficiency and relative distributions of heat loss mechanisms, the small scale optimal design was scaled to accept 1 MW solar power. The window aspect ratio is maintained identical to that utilized in the existing laboratory-scale receiver and aperture surface area is scaled proportionally to the solar input. The shape of the solar flux profile as a function of dimensionless position on the window surface is identical to that employed in the models described above. All receiver dimensions are modified in relation to the window size and flow rates are scaled linearly in accordance with the solar input. The resulting tube radius exceeds that of the optimal laboratory-scale design by a factor of 11.2. Though flow in the small-scale design is characterized by a Reynolds number less than 500, this value increases to 1500-6000 at the large scale depending on operating conditions. Thus computational fluid dynamics models for the large-scale receiver are carried out with a

standard k- $\varepsilon$  closure model and the Reynolds averaged Navier-Stokes equations [25] in place of the simple laminar flow model employed in the small-scale design.

Resultant calculations of receiver efficiency, reaction conversion, tube temperatures at the horizontal center plane, and heat loss mechanisms for the design in Figure 7.12 at both 8 kW and 1 MW are provided in Table 7.10. Temperatures at the front and back external surfaces of the center tube are illustrated in Figure 7.14 as a function of the dimensionless vertical position with y/L = 0 defined at the top of the tube.

	8 kW	1 MW
η (%)	35.5	41.2
$X_{max}$ / $X_{avg}$ (%)	61 / 51	66 / 62
$\eta_1$ (%)	69.6	67.3
$\eta_2$ (%)	51.1	59.9
Center tube <i>T<sub>front</sub></i> (K)	1920	1898
Center tube $T_{back}$ (K)	1470	1293
Outer tube $T_{max}$ (K)	1742	1750
<u>Heat losses</u> (% of solar input)		
Solar reflection	10.2	10.5
Transmission at window	15.7	19.5
Net absorption at cavity wall	20.1	8.3
Tube conduction	3.3	1.8

Table 7.10: Performance of the optimal small-scale absorbing cavityreceiver configuration at 8 kW and 1 MW

The solar-to-chemical efficiency is predicted to reach 41% at 1 MW, though the linearly scaled flow rates from the 8 kW design may not be optimal at this scale. Maximum tube temperatures are similar with an increased center tube front / back temperature discrepancy at 1 MW arising from the large tube radius. The relative distribution between conduction and emission losses is analogous at each scale, but the emission losses by transmission increase from 16% in the 8 kW
design to 20% in the 1 MW design whereas those due to net cavity wall absorption decrease from 20% to 8% owing to the diminished surface-to-volume ratio. Figure 7.14 indicates that the nondimensionalized heated length is similar for both 8 kW and 1 MW designs. The increase in efficiency at the large scale is predominantly attributed to enhanced absorption efficiency due to diminished cavity wall absorption losses and utilization of absorbed energy is equivalently effective at each scale. The large scale design exhibits an analogous relative distribution between heat loss mechanisms compared to the small scale design and, as such, optimal designs at each scale are likely characterized by similar tube configurations.



Figure 7.14: Center tube front and back external surface temperature as a function of dimensionless vertical position for 8 kW and 1 MW

### 7.9 Conclusions

The effects of fifteen distinct parameters describing receiver geometry, cavity size, and operating conditions on solar-to-chemical efficiency of an absorbing cavity receiver were examined by means of a series of fractional factorial and central composite design studies. All designs were evaluated for steam gasification of acetylene black via a computational model

coupling heat, mass, momentum, chemical reaction, and radiation phenomena similar to that detailed in Chapter 5. The specularly reflecting cavity wall with spectral directional optical properties described in Chapters 5 and 6 was replaced with a diffuse gray boundary and heat transfer through the surrounding insulating layer was approximated with one-dimensional conduction. Optimal designs were selected on the basis of the solar flux profile generated by the High Flux Solar Furnace at the National Renewable Energy Laboratory with solar power restricted to 8 kW. The insulated, absorbing cavity wall reached temperatures higher than those permitted by a reflective surface and, through thermal emission from the heated wall, produced a longer heated tube length, improved uniformity in tube temperature distributions and, correspondingly, higher average reaction conversion and receiver efficiency than observed with a reflective cavity boundary. The dominant heat loss mechanism shifted from tube conduction in reflective cavity designs to emission in absorbing cavity receiver performance.

Variability in efficiency between individual receiver designs was dominated by cavity radius, solar power, and carbon feed rate. A similar subset of factors describing geometric tube configurations impacted both absorbing and reflective designs, but the nature of these effects was entirely distinct. Absorbing cavity configurations were comparatively less sensitive to spatial tube positions than reflective cavity designs and factors producing modification in spatial positioning alone without introducing variability in size or number of tubes did not impact receiver performance. Unlike reflective cavity designs, positioning tubes outside of the initial solar beam only detrimentally impacted receiver performance at excessively large cavity size. Optimal absorbing cavity designs maximized tube radius thereby leading to long residence time, minimal solar energy incident on the cavity wall, and high external tube surface area. Tubes were sized such that the total external surface area was independent of the maximum number of tubes and, as such, the nominal plug flow residence time without gas expansion in any given tube increased as the number of tubes decreased.

Optimal designs typically contained large tubes arranged in a semicircle around the back cavity wall and the unconstrained optimum solar-to-chemical efficiency determined from calculations in this study was 35.9% with an 8 kW solar input. A more physically realistic receiver design placed constraints on the maximum allowable surface temperature, and tube temperatures were restricted to 1900 K while maintaining 35.4% efficiency. The temperature constraint was principally enforced by modifications in cavity size which created physical separation between the tube array the focal point of the solar concentration system. Improvements in receiver performance above that predicted for the existing configuration arose primarily from comparatively higher net absorption efficiency and longer residence time. The optimal small-scale design was scaled linearly to accept 1 MW solar power and the predicted efficiency for the large-scale design exceeded 41% despite potentially unoptimized feed rates. The large scale design exhibited an analogous relative distribution between heat loss mechanisms compared to the small scale design and, as a result, optimal designs at each scale are likely characterized by similar tube configurations.

#### Nomenclature

A	total tube surface area per unit length
$C_{feed}$	total carbon feed rate
$f_l$	parameter describing offset of the back of the tube array toward the window
$f_2$	parameter describing tube semicircle radius
$f_o$	parameter describing offset of entire tube array toward window
$f_r$	ratio of center tube cross-sectional area to outer tube cross-sectional area

$f_s$	parameter describing tube staggering
$h_{cav}$	cavity height
k	thermal conductivity
Lins	insulation thickness
N <sub>max</sub>	maximum number of tubes
$q''_w$	conductive heat flux at wall
$Q_{reaction}$	energy used to carry out the endothermic reaction
$Q_s$	solar power (kW)
$Q_{tubes}$	energy transferred into the tube solid material
r	correlation coefficient
<i>r<sub>cav</sub></i>	cavity radius
$r_t$	tube radius
$R_I$	standard inert gas flow rate / individual tube volume in front of the aperture
R <sub>steam</sub>	molar ratio of steam to carbon feed rate
Т	temperature (K)
$T_{ext}$	external insulation temperature
$T_w$	wall temperature (K)
X	fractional carbon conversion
η	solar-to-chemical receiver efficiency
$\eta_1$	ratio of energy used for reaction to energy transferred into tubes
$\eta_2$	ratio of energy transferred into tubes to solar energy input
$\eta_{max,C}$	receiver efficiency at 100% carbon conversion
$\eta_{max,rad}$	receiver efficiency if all solar energy not lost by emission or reflection is utilized
$ heta_c$	angular extent of tube array measured from cavity centroid

# References

1. Abanades, S., Charvin, P., and Flamant, G., Design and simulation of a solar chemical reactor for the thermal reduction of metal oxides: Case study of zinc oxide dissociation. *Chemical Engineering Science*, 2007. **62**(22): p. 6323-6333.

- 2. Melchior, T., Perkins, C., Weimer, A.W., and Steinfeld, A., A cavity-receiver containing a tubular absorber for high-temperature thermochemical processing using concentrated solar energy. *International Journal of Thermal Sciences*, 2008. **47**(11): p. 1496-1503.
- 3. Palumbo, R., Keunecke, M., Moller, S., and Steinfeld, A., Reflections on the design of solar thermal chemical reactors: thoughts in transformation. *Energy*, 2004. **29**(5-6): p. 727-744.
- 4. Siegel, N.P., Ho, C.K., Khalsa, S.S., and Kolb, G.J., Development and Evaluation of a Prototype Solid Particle Receiver: On-Sun Testing and Model Validation. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(2).
- 5. Wieckert, C., Palumbo, R., and Frommherz, U., A two-cavity reactor for solar chemical processes: heat transfer model and application to carbothermic reduction of ZnO. *Energy*, 2004. **29**(5-6): p. 771-787.
- 6. Z'Graggen, A. and Steinfeld, A., Hydrogen production by steam-gasification of carbonaceous materials using concentrated solar energy V. Reactor modeling, optimization, and scale-up. *International Journal of Hydrogen Energy*, 2008. **33**(20): p. 5484-5492.
- 7. Lichty, P., Perkins, C., Woodruff, B., Bingham, C., and Weimer, A., Rapid High Temperature Solar Thermal Biomass Gasification in a Prototype Cavity Reactor. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(1).
- 8. Steinfeld, A. and Fletcher, E.A., A Solar Receiver-Reactor with Specularly Reflecting Walls for High-Temperature Thermoelectrochemical and Thermochemical Processes. *Energy*, 1988. **13**(4): p. 301-311.
- 9. Schunk, L.O., Lipinski, W., and Steinfeld, A., Heat transfer model of a solar receiverreactor for the thermal dissociation of ZnO-Experimental validation at 10 kW and scaleup to 1 MW. *Chemical Engineering Journal*, 2009. **150**(2-3): p. 502-508.
- 10. Petrasch, J., Osch, P., and Steinfeld, A., Dynamics and control of solar thermochemical reactors. *Chemical Engineering Journal*, 2009. **145**(3): p. 362-370.
- 11. Petrasch, J. and Steinfeld, A., Dynamics of a solar thermochemical reactor for steamreforming of methane. *Chemical Engineering Science*, 2007. **62**(16): p. 4214-4228.
- 12. Muller, R., Lipinski, W., and Steinfeld, A., Transient heat transfer in a directly-irradiated solar chemical reactor for the thermal dissociation of ZnO. *Applied Thermal Engineering*, 2008. **28**(5-6): p. 524-531.
- 13. Dahl, J.K., Buechler, K.J., Weimer, A.W., Lewandowski, A., and Bingham, C., Solarthermal dissociation of methane in a fluid-wall aerosol flow reactor. *International Journal of Hydrogen Energy*, 2004. **29**(7): p. 725-736.

- 14. Hirsch, D. and Steinfeld, A., Radiative transfer in a solar chemical reactor for the coproduction of hydrogen and carbon by thermal decomposition of methane. *Chemical Engineering Science*, 2004. **59**(24): p. 5771-5778.
- 15. Meier, A., Bonaldi, E., Cella, G.M., Lipinski, W., Wuillemin, D., and Palumbo, R., Design and experimental investigation of a horizontal rotary reactor for the solar thermal production of lime. *Energy*, 2004. **29**(5-6): p. 811-821.
- 16. Melchior, T., Perkins, C., Lichty, P., Weimer, A.W., and Steinfeld, A., Solar-driven biochar gasification in a particle-flow reactor. *Chemical Engineering and Processing*, 2009. **48**(8): p. 1279-1287.
- 17. Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., Hydrogen production from solar thermal dissociation of natural gas: development of a 10 kW solar chemical reactor prototype. *Solar Energy*, 2009. **83**(9): p. 1599-1610.
- Schaffner, B., Meier, A., Wuillemin, D., Hoffelner, W., and Steinfeld, A., Recycling of hazardous solid waste material using high-temperature solar process heat. 2. Reactor design and experimentation. *Environmental Science & Technology*, 2003. 37(1): p. 165-170.
- 19. Tescari, S., Mazet, N., and Neveu, P., Constructal method to optimize solar thermochemical reactor design. *Solar Energy*, 2010. **84**(9): p. 1555-1566.
- 20. Tescari, S., Mazet, N., Neveu, P., and Abanades, S., Optimization Model for Solar Thermochemical Reactor: Efficiency Increase by a Nonuniform Heat Sink Distribution. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2011. **133**(3).
- 21. Melchior, T. and Steinfeld, A., Radiative transfer within a cylindrical cavity with diffusely/specularly reflecting inner walls containing an array of tubular absorbers. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2008. **130**(2).
- Haussener, S., Hirsch, D., Perkins, C., Weimer, A., Lewandowski, A., and Steinfeld, A., Modeling of a Multitube High-Temperature Solar Thermochemical Reactor for Hydrogen Production. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2009. 131(2).
- 23. Montgomery, D., *Design and Analysis of Experiments*. 6th ed. 2005, New York: John Wiley and Sons.
- 24. Trommer, D., *Thermodynamic and Kinetic Analyses of the Solar Thermal Gasification of Petroleum Coke*. 2006, Swiss Federal Institute of Technology: Zurich.
- 25. Versteeg, H.K. and Malalasekera, W., *An Introduction to Computational Fluid Dynamics*. 2<sup>nd</sup> ed. 2007, Harlow, England: Pearson Education.

# **Chapter VIII**

# **Conclusions and Future Directions**

#### 8.1 Summary and Conclusions

A three-dimensional, steady state computational model coupling radiative transfer with fluid flow, heat transfer, mass transfer, and chemical reaction kinetics was developed for a solar receiver consisting of an array of five tubes enclosed within a specularly reflective cylindrical cavity with a windowed or windowless aperture. This model was experimentally validated and utilized to both assess performance of the existing design and identify optimally efficient receiver configurations. Radiative energy was separated into two components consisting of: (1) solar energy introduced through the receiver aperture and (2) energy emitted by heated surfaces within the enclosure. A Monte Carlo model was developed for the solar component under the assumption of non-attenuating media present in the cavity space in order to assess the accuracy of approximate solution methods for the complex integro-differential equations describing radiative transfer. The Monte Carlo model is valid for both specularly and diffusely reflecting surfaces with spectral directional optical properties for specular surfaces computed via electromagnetic theory. Calculation of known configuration factors via the Monte Carlo model suggested that physically realistic solutions require at least 10<sup>7</sup> rays.

Approximate finite volume radiation models were evaluated in two-dimensional slices of two closed cavity solar receiver configurations via comparison with corresponding Monte Carlo calculations. Two-dimensional spatial grids for the finite volume method contained 2,300-133,000 mesh elements with angular grids defined by  $(N_{\theta} \times N_{\phi}) = (5x5)$ , (15x15), or (25x25) where  $N_{\theta}$  and  $N_{\phi}$  represent the number of divisions in each the zenith and azimuth angle per octant of space. Energy introduced at the aperture was treated as either collimated, diffuse or uniform with a specified cone angle and quantitatively accurate finite volume solutions either required highly refined angular and spatial grids, or were not possible due to false scattering and ray concentration errors. These errors were exacerbated by specularly reflective boundaries and collimated radiative energy. Ray concentration errors were predominant on angular grids specified by  $(N_{\theta} x N_{\phi}) = (5x5)$  whereas both ray concentration and false scattering errors were evident on angular grids specified by  $(N_{\theta} x N_{\phi}) = (15x15)$  or (25x25). Finite volume solutions exhibited artificial spreading of the solar beam resulting in physically unrealistic peaks of solar energy incident on tube surfaces located predominantly outside the extent of the solar beam. Solar absorption was overestimated by as much as a factor of ten in these locations. These approximations improved as the character of the incident solar energy shifted from collimated to diffuse, but even calculations for diffuse energy necessitated highly refined angular and spatial grids thereby producing prohibitively large computational requirements for full threedimensional simulations. On the contrary, finite volume solutions for radiative energy emitted diffusely by tube surfaces were sufficiently accurate on coarse angular and spatial grids. Though local oscillations in energy flux profiles occasionally arose from interactions between ray concentration and false scattering errors, the quantity of energy absorbed by a given surface was accurate to within 1% of the total emitted energy with any angular or spatial grid.

The solar radiation solution can be entirely decoupled from all other heat transfer phenomena occurring in the receiver when the spectral surface absorptivity is independent of temperature. Emitted radiation, on the other hand, is strongly dependent on surface optical properties, temperatures and, correspondingly, all convection and conduction phenomena occurring in the receiver. These results suggest an optimal hybrid approach employing the Monte Carlo method for the solar energy and the finite volume method for the emitted energy, thereby retaining both the accuracy of the Monte Carlo technique for the solar component and the compatibility of the finite volume technique with control-volume based computational fluid dynamics heat transfer models. Based on this radiation modeling strategy, a theoretical model was developed for gasification of nano-sized acetylene black particles in an existing reflective cavity solar receiver. The spatial flux profile and direction of solar energy entering the receiver was characterized as a function of solar input via ray trace modeling of the High Flux Solar Furnace at the National Renewable Energy Laboratory (NREL). These profiles were converted to probability distributions for specification of initial ray position and direction in the Monte Carlo model, the output of which takes the form of spatial profiles of solar energy absorbed by each receiver surface. More than 90% of solar energy absorption occurred prior to reflection at the cavity wall, with the center tube absorbing two to four times more solar energy than each outlying tube.

The finite volume model describing diffusely emitted energy was solved simultaneously and on the same spatial mesh as a three dimensional steady state computational fluid dynamics model describing the heat, mass, momentum and chemical reaction processes occurring in the receiver. Momentum and thermal Stokes numbers were on the order of 10<sup>-5</sup> with convective and radiative Biot numbers ranging from 10<sup>-7</sup>-10<sup>-2</sup> for the 42 nm acetylene black particles considered in this study. As such, an Eulerian-Eulerian two-phase model was simplified to a single fluid mixture model with particle transport dictated by an aerosol population balance incorporating convection, Brownian motion, and thermophoretic diffusion. Internal heat and mass transfer limitations were disregarded in view of an estimated particle effectiveness factor which exceeded 99% under all realistic reaction conditions. Mie theory calculations indicated that the spectral extinction coefficient for the particle cloud was dominated by absorption with nearly negligible contribution from scattering.

Maximum temperatures of 1813 K, 1343 K, and 1546 K were predicted with a 6 kW solar input for the center, front east, and back east tubes respectively, with corresponding carbon conversion of 40%, 2.5%, and 9.2%. Average residence time was on the order of 1 s with more than 80% of reaction conversion occurring within 15% of the tube length. Predicted temperature profiles were highly non-uniform, particularly at the front of the center tube where temperature varied by 450 K over a mere 5 cm tube length. Front and back surface temperatures differed by as much as 340 K for a 6 kW solar power input, with gas/particle mixture temperature tracking closely to that of the surrounding wall owing to radiative exchange between the heated wall and entrained carbon particles. Predicted solar-to-chemical receiver efficiency ranged from 1-4% for the existing design depending on operating conditions. Emission losses accounted for 11-25% of the solar input whereas conductive heat losses accounted for 55-69% and occurred predominantly via conduction along the tube length toward upper and lower cooling zones. Low efficiency was largely attributed to poor utilization of absorbed solar energy, particularly in outlying tubes which absorbed 43% of the solar energy but failed to reach sufficient temperatures to carry out the reaction to a significant extent. Uncertainty in property inputs, assumed to be at most 15% of nominal values, altered predicted maximum temperature, fractional conversion, and fractional receiver efficiency by at most 58 K, 0.06, and 0.01 and model predictions were most sensitive to variability in tube thermal conductivity and cavity reflectivity. Temperature profiles predicted by the numerical model agreed with on-sun experimental data within, on average, 44 K (4%) and 21 K (2%) for temperature ranges of 600-1700 K and 700-1400 K measured with

silicon carbide and Inconel tubes, respectively. Fractional conversion of acetylene black to CO and  $CO_2$  was measured in the center tube and resulting values were well within the range predicted by the theoretical model utilizing kinetic parameters available in the literature.

The effects of fifteen distinct parameters describing receiver geometry, cavity size, and operating conditions were examined by means of a series of fractional factorial and central composite design studies for both insulated absorbing and cooled reflective cavity configurations. All designs were evaluated on the basis of receiver solar-to-chemical efficiency. High efficiency was only achievable with a large carbon feed rate, more than 7 kW solar power, and small cavity radius regardless of tube configuration, though practical constraints on maximal allowable temperature or absorbed solar energy flux dictated a realistic minimal cavity size.

Calculations for a reflective cavity design indicated that all tubes positioned outside of the initial solar beam failed to reach temperatures high enough to carry out the reaction and instead functioned as heat sinks conducting energy toward cooling zones encircling the receiver. Reflective cavity designs were, in general, dominated by conductive rather than emissive losses, and maximization of absorbed energy utilization via minimization of conduction losses was a more effective means of improving receiver performance than maximization of net absorption efficiency. Ideal tube configurations allowed a portion of the solar energy to strike the cavity wall. The resulting specularly reflected solar energy was preferentially directed toward the back of the tube array and enhanced uniformity of front/back temperature distributions. An optimal intermediate tube radius arose from competing effects pertaining to wall temperature uniformity and fluid velocity or residence time. In the limit of zero fluid velocity, radiative exchange between tube walls and entrained carbon particles dictated that the centerline temperature reached, at best, a value intermediate to that attained at the front and back walls. Designs with small tubes allowed more solar reflection and produced the highest hypothetical centerline temperature in the zero-flow limit, but approach of the actual value to this limit was restricted by rapid gas velocity.

The best receiver configurations consisted of an array of three tubes situated near the back cavity wall and positioned entirely within the solar beam. The unconstrained optimum predicted solar-to-chemical efficiency was 13.2% for a reflective cavity receiver accepting up to 8 kW solar power. The maximum achievable efficiency was reduced to 12.3% with solar flux absorption restricted to at most 1000 kW/m<sup>2</sup>. Solar flux constraints were imposed via modifications in cavity size with little variation in tube array configuration. Compared to the existing design, optimal designs were characterized by improved uniformity in absorbed solar energy and surface temperature distributions, longer heated tube length, diminished conduction losses, and improved utilization of absorbed energy despite lower net absorption efficiency and increased emission losses. Net absorption by the tube array accounted for nearly 50% of the solar input in the existing design, but only 10% of this energy was utilized for the endothermic chemical reaction. Under identical conditions, net absorption in the optimal design accounted for only 41% of the solar input, but nearly 30% of this energy was utilized for reaction. Linear geometric scaling of the optimal design to accept 1 MW solar power resulted in a predicted 22% solar-to-chemical efficiency despite potentially suboptimal feed rates. However, a shift in the dominant mode of heat loss from conduction in the small-scale design to emission in the large scale design suggested that the geometrical configuration of an optimized large scale reflective cavity receiver may differ from that determined on a small scale.

An insulated, absorbing cavity wall reached temperatures higher than those permitted by a reflective surface and, through thermal emission from the heated wall, produced a longer heated tube length, improved uniformity in tube temperature distributions and, correspondingly, higher average reaction conversion and receiver efficiency than observed with a reflective cavity boundary. Computational evaluation of the existing design with an insulated, absorbing cavity wall indicated less than 5% loss of the solar input by tube conduction with more than 60% loss by emission through either transmission out of the aperture or net absorption at the cavity surface. Though a similar subset of parameters describing spatial tube configurations impacted both absorbing and reflective designs, the shift in the dominant mode of heat loss altered the nature of these effects. Enhanced temperature uniformity arising from cavity wall thermal emission rendered absorbing cavity configurations relatively impervious to tube positioning, and thus parameters relating purely to tube location were inconsequential. Optimal designs contained large tube radii leading to maximal residence time, tube surface area, and solar absorption efficiency. Solar incidence on the cavity wall was correspondingly minimized as, unlike the behavior observed with a specularly reflective cavity boundary, diffusely reflected or re-emitted energy was not preferentially directed toward the tube array.

The optimal absorbing cavity design accepting up to 8 kW solar power consisted of three large tubes placed in a semicircle at the back cavity wall and produced a solar-to-chemical efficiency exceeding 35%. This value only marginally exceeded the predicted 29% efficiency for the existing tube configuration under identical operating conditions. However, the optimal configuration remained within a physically realistic range of operating parameters imposed by the tube materials and reduced the maximum temperature and absorbed solar flux by 140 K and 600 kW/m<sup>2</sup>, respectively, compared to the existing configuration. Linear geometric scaling of the optimal design to accept 1 MW solar power resulted in a predicted 41% solar-to-chemical efficiency despite potentially suboptimal feed rates. Analogous relative distributions between

heat loss mechanisms were observed for both small- and large-scale designs suggesting similar optimal configurations at either scale.

Computational results described in this study revealed that an indirectly irradiated multiple tube aerosol flow receiver is theoretically capable of achieving high solar-to-chemical efficiency compared to alternative designs detailed in the literature. An insulated, absorbing cavity configuration performed markedly better than a reflective cavity configuration at a small scale. While calculations suggested that this distinction was less notable at an industrial scale, additional advantages related to large thermal mass and correspondingly reduced sensitivity to transient variations in solar input render the absorbing cavity configuration preferable for continuous operation.

#### 8.2 Suggested future research directions

The intent of this study was to develop the structure of a model coupling radiative transfer with fluid flow, heat transfer, mass transfer and chemical reaction kinetics thereby providing a framework for assessment and optimization of receiver performance. Detailed understanding of intrinsic chemical phenomena is required to achieve accurate simulation results and, as this has not yet been developed for biomass pyrolysis and gasification processes at elevated temperatures, calculations were carried out for gasification of pure carbon. Alternative chemical reaction models may be incorporated within the framework described herein once predictive kinetic parameters become available. The current model was restricted to treatment of micron or nano-sized particles both for simplicity and to place special emphasis on development of radiation and heat transfer models. Physically realistic biomass particles are comparatively more massive and would require both consideration of internal heat and mass transfer processes

and replacement of the single phase mixture model with a discrete Lagrangian treatment for the particulate phase. Auxiliary enhancement to the current model for both biomass and metal oxide species could include conversion-dependent physical and optical particle properties and complex intrinsic kinetic mechanisms including, for example, product inhibition and reversible reactions. Analysis of receiver performance and assessment of optimal receiver configurations for disparate chemical processes would be of interest as the sensitivity of optimal receiver design to the identity, kinetic rate, and temperature range of the chemical process remains unknown.

The current work utilized studies based on fractional factorial designs to point toward a region of optimal performance with minimal computational requirements. Approximate optimal designs were selected from second-order response surface models for a subset of five parameters. Gradient based optimization techniques could provide a more comprehensive method of assessing optimal configurations and operating conditions on the basis of all parameters, albeit with a substantial increase in computational requirements. While the calculations provided herein may identify the main features of optimal designs, gradient based techniques could be utilized to fine-tune receiver performance. Furthermore, optimization of industrially-scaled designs should be carried out independently from the calculations detailed here, particularly for reflective cavity configurations for which an increase in physical size produced a shift in dominant heat loss mechanisms. Large-scale reflective cavity receivers began to exhibit characteristics reminiscent of absorbing cavity designs. Thus even though reflective cavity receivers are not likely to be industrially relevant, it may be of interest from a theoretical standpoint to ascertain if optimal large-scale reflective and absorbing cavity designs share similar features distinct from those characterizing optimal small-scale reflective cavity designs.

The current study focused on model development for an aerosol flow configuration with optimization calculations restricted to a single specified flux profile, simple tube and cavity shapes, and tubular arrays which consistently placed a tube in direct alignment with the center of the window. Though the aerosol flow configuration allows for kinetically controlled reactions with rapid heat and mass transfer processes, it also produces limited residence time, particularly for the large feed rates required to match the endothermic reaction heat sink to the solar input. An analogous design could be operated in a packed bed configuration, an option which may be of practical interest for metal oxide thermochemical cycles in which the entire cycle may, theoretically, be carried out without requiring replacement of the reactive material.

Receiver performance, particularly that for reflective cavity designs, was strongly impacted by tube positions relative to the solar beam. While the current study took the approach of optimizing tube positioning for a fixed solar profile, independent assessment of an ideal flux profile may also provide a means of improving receiver performance. The solar flux profile is adjustable via design of, and modifications to, the array of mirrors comprising the solar concentration system. Thus it may be possible to carry out calculations selecting both an optimal profile and an optimal tube array simultaneously. At minimum, analysis of optimal design sensitivity to the shape and direction of the solar beam would be of interest. Similarly, as reflective cavity receiver efficiency was typically restricted by low temperature achieved at the back side of the tube array, any additional modifications which increase the solar incidence on the back of the tubes may further improve receiver performance. An elliptical cavity shape could be considered along with removal of the center tube though, based on the geometric configuration of the receiver, this may result in substantial reflection losses as well as an excessive heat load on the back cavity wall. Finally, optimal designs identified through this study point to an ideal range of conditions pushing temperatures and absorbed solar flux near the operating limit of silicon carbide tubes. Continuous operation with a concentrated solar input is characteristically more unforgiving than traditionally-defined continuous operation due to highly non-uniform flux absorption and frequent interruptions in the power source due to transient environmental variables. Thus, while silicon carbide is currently the material of choice given its high operating temperature and superior resistance to thermal shock and oxidation, further investigation into materials for receiver construction may prove to be essential.

#### BIBLIOGRAPHY

Annual Energy Review 2010. 2011: U.S. Energy Information Administration, Washington DC.

- Assessment of the World Bank Group / GEF Strategy for the Market Development of Concentrating Solar Thermal Power. 2006: World Bank, Washington DC.
- Abanades, S., Charvin, P., Flamant, G., and Neveu, P., Screening of water-splitting thermochemical cycles potentially attractive for hydrogen production by concentrated solar energy. *Energy*, 2006. **31**(14): p. 2805-2822.
- Abanades, S. and Flamant, G., Thermochemical hydrogen production from a two-step solardriven water-splitting cycle based on cerium oxides. *Solar Energy*, 2006. **80**(12): p. 1611-1623.
- Abanades, S., Charvin, P., and Flamant, G., Design and simulation of a solar chemical reactor for the thermal reduction of metal oxides: Case study of zinc oxide dissociation. *Chemical Engineering Science*, 2007. **62**(22): p. 6323-6333.
- Abanades, S., Charvin, P., Lemont, F., and Flamant, G., Novel two-step SnO2/Sno watersplitting cycle for solar thermochemical production of hydrogen. *International Journal of Hydrogen Energy*, 2008. **33**(21): p. 6021-6030.
- Abanades, S., Legal, A., Cordier, A., Peraudeau, G., Flamant, G., and Julbe, A., Investigation of reactive cerium-based oxides for H(2) production by thermochemical two-step watersplitting. *Journal of Materials Science*, 2010. 45(15): p. 4163-4173.
- Abraham, B.M. and Schreine.F, General Principles Underlying Chemical Cycles Which Thermally Decompose Water into Elements. *Industrial & Engineering Chemistry Fundamentals*, 1974. **13**(4): p. 305-310.
- Adanez, J. and Labiano, F.G., Modeling of Moving-Bed Coal Gasifiers. *Industrial & Engineering Chemistry Research*, 1990. **29**(10): p. 2079-2088.
- Agrafiotis, C., Roeb, M., Konstandopoulos, A.G., Nalbandian, L., Zaspalis, V.T., Sattler, C., Stobbe, P., and Steele, A.M., Solar water splitting for hydrogen production with monolithic reactors. *Solar Energy*, 2005. **79**(4): p. 409-421.
- Allendorf, M.D., Diver, R.B., Siegel, N.P., and Miller, J.E., Two-Step Water Splitting Using Mixed-Metal Ferrites: Thermodynamic Analysis and Characterization of Synthesized Materials. *Energy & Fuels*, 2008. 22(6): p. 4115-4124.
- Baek, S.W., Byun, D.Y., and Kang, S.J., The combined Monte-Carlo and finite-volume method for radiation in a two-dimensional irregular geometry. *International Journal of Heat and Mass Transfer*, 2000. **43**(13): p. 2337-2344.

- Balat, M., Mechanisms of thermochemical biomass conversion processes. Part 2: Reactions of gasification. *Energy Sources Part a-Recovery Utilization and Environmental Effects*, 2008. **30**(7): p. 636-648.
- Bale, C., Chartrand, P., Degterov, S.A., Eriksson, G., Hack, K., Ben Mahfoud, R., Melancon, J., Pelton, A.D., and Petersen, S., FactSage thermochemical software and databases. *Calphad-Computer Coupling of Phase Diagrams and Thermochemistry*, 2002. 26(2): p. 189-228.
- Barrio, M., Goble, B., Risnes, H., Henriksen, U., Hustad, J.E., and Sorensen, L.H., Steam gasification of wood char and the effect oh hydrogen inhibition on the chemical kinetics, in Progress in thermochemical biomass conversion, A. V. Bridgwater, Editor. 2001, Blackwell Science Ltd.: Oxford. p. 32-46.
- Bharadwaj, A., Baxter, L.L., and Robinson, A.L., Effects of intraparticle heat and mass transfer on biomass devolatilization: Experimental results and model predictions. *Energy & Fuels*, 2004. 18(4): p. 1021-1031.
- Bhattacharya, A., Salam, L., Dudukovic, M.P., and Joseph, B., Experimental and Modeling Studies in Fixed-Bed Char Gasification. *Industrial & Engineering Chemistry Process Design* and Development, 1986. 25(4): p. 988-996.
- Biba, V., Macak, J., Klose, E., and Malecha, J., Mathematical-Model for Gasification of Coal under Pressure. *Industrial & Engineering Chemistry Process Design and Development*, 1978. 17(1): p. 92-98.
- Bilgen, E., Ducarroir, M., Foex, M., Sibieude, F., and Trombe, F., Use of Solar-Energy for Direct and 2-Step Water Decomposition Cycles. *International Journal of Hydrogen Energy*, 1977. 2(3): p. 251-257.
- Bindoff, N.L., Willebrand, J., Artale, V., Cazenave, A., Gregory, J., Gulev, S., Hanawa, K., Le Quere, C., Levitus, S., Nojiri, Y., Shum, C.K., Talley, L.D., and Unnikrishnan, A., Observations: Oceanic Climate Change and Sea Level, in Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, S. Soloman, D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Avery, M. Tignor, and H.L. Miller, Editors. 2007, Cambridge University Press: Cambridge.
- Bird, R.B., Stewart, W.E., and N., L.E., *Transport Phenomena*. 2<sup>nd</sup> ed. 2002, New York: John Wiley and Sons, Inc.
- Blackwood, J.D. and Mcgrory, F., The Carbon-Steam Reaction at High Pressure. *Australian Journal of Chemistry*, 1958. **11**(1): p. 16-33.
- Bohren, C.F. and Huffman, D.R., *Absorption and Scattering of Light by Small Particles*. 1983, New York: Wiley.

- Brockmann, H., Analytic angle factors for the radiant interchange among the surface elements of two concetnric cylinders. *International Journal of Heat and Mass Transfer*, 1994. **37**(7): p. 1095-1100.
- Brown, A.L., Dayton, D.C., Nimlos, M.R., and Daily, J.W., Design and characterization of an entrained flow reactor for the study of biomass pyrolysis chemistry at high heating rates. *Energy & Fuels*, 2001. 15(5): p. 1276-1285.
- Brown, A.L., Dayton, D.C., and Daily, J.W., A study of cellulose pyrolysis chemistry and global kinetics at high heating rates. *Energy & Fuels*, 2001. **15**(5): p. 1286-1294.
- Bustamante, F., Enick, R.M., Cugini, A.V., Killmeyer, R.P., Howard, B.H., Rothenberger, K.S., Ciocco, M.V., and Morreale, B.D., High-temperature kinetics of the homogeneous reverse water-gas shift reaction. *Aiche Journal*, 2004. **50**(5): p. 1028-1041.
- Bustamante, F., Enick, R.M., Killmeyer, R.P., Howard, B.H., Rothenberger, K.S., Cugini, A.V., Morreale, B.D., and Ciocco, M.V., Uncatalyzed and wall-catalyzed forward water-gas shift reaction kinetics. *Aiche Journal*, 2005. **51**(5): p. 1440-1454.
- Byun, D.Y., Baek, S.W., and Kim, M.Y., Thermal radiation in a discretely heated irregular geometry using the Monte-Carlo, finite volume, and modified discrete ordinates interpolation method. *Numerical Heat Transfer Part a-Applications*, 2000. **37**(1): p. 1-18.
- Caram, H.S. and Amundson, N.R., Fluidized-Bed Gasification Reactor Modeling .1. Model Description and Numerical Results for a Single Bed. *Industrial & Engineering Chemistry Process Design and Development*, 1979. 18(1): p. 80-96.
- Chai, J.C., Lee, H.S., and Patankar, S.V., Ray Effect and False Scattering in the Discrete Ordinates Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. **24**(4): p. 373-389.
- Chai, J.C., Hsu, P.F., and Lam, Y.C., Three-dimensional transient radiative transfer modeling using the finite-volume method. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2004. 86(3): p. 299-313.
- Chan, W.C.R., Kelbon, M., and Krieger, B.B., Modeling and Experimental-Verification of Physical and Chemical Processes during Pyrolysis of a Large Biomass Particle. *Fuel*, 1985. 64(11): p. 1505-1513.
- Chan, W.C.R., Kelbon, M., and Kriegerbrockett, B., Single-Particle Biomass Pyrolysis -Correlations of Reaction-Products with Process Conditions. *Industrial & Engineering Chemistry Research*, 1988. 27(12): p. 2261-2275.
- Charvin, P., Abanades, S., Flamant, G., and Lemort, F., Two-step water splitting thermochemical cycle based on iron oxide redox pair for solar hydrogen production. *Energy*, 2007. **32**(7): p. 1124-1133.

- Charvin, P., Abanades, S., Lemont, F., and Flamant, G., Experimental study of SnO2/SnO/Sn thermochemical systems for solar production of hydrogen. *Aiche Journal*, 2008. **54**(10): p. 2759-2767.
- Chen, H.J., Chen, Y.T., Hsieh, H.T., and Siegel, N., Computational fluid dynamics modeling of gas-particle flow within a solid-particle solar receiver. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2007. **129**(2): p. 160-170.
- Chueh, W.C., Falter, C., Abbott, M., Scipio, D., Furler, P., Haile, S.M., and Steinfeld, A., High-Flux Solar-Driven Thermochemical Dissociation of CO(2) and H(2)O Using Nonstoichiometric Ceria. *Science*, 2010. **330**(6012): p. 1797-1801.
- Chui, E.H. and Raithby, G.D., Computation of Radiant-Heat Transfer on a Nonorthogonal Mesh Using the Finite-Volume Method. *Numerical Heat Transfer Part B-Fundamentals*, 1993. 23(3): p. 269-288.
- Churchill, S.W. and Bernstein, M., Correlating Equation for Forced-Convection from Gases and Liquids to a Circular-Cylinder in Cross-Flow. *Journal of Heat Transfer-Transactions of the Asme*, 1977. **99**(2): p. 300-306.
- Coelho, P.J., The role of ray effects and false scattering on the accuracy of the standard and modified discrete ordinates methods. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2002. **73**(2-5): p. 231-238.
- Corlett, R.C., Direct Monte Carlo Calculation of Radiative Heat Transfer in Vacuum. *Journal of Heat Transfer*, 1966. **88**(4): p. 376.
- Crosbie, A.L. and Davidson, G.W., Dirac-Delta Function Approximations to the Scattering Phase Function. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1985. **33**(4): p. 391-409.
- Dahl, J.K., Buechler, K.J., Weimer, A.W., Lewandowski, A., and Bingham, C., Solar-thermal dissociation of methane in a fluid-wall aerosol flow reactor. *International Journal of Hydrogen Energy*, 2004. 29(7): p. 725-736.
- Dalzell, W.H. and Sarofim, A.F., Optical Constants of Soot and Their Application to Heat-Flux Calculations. *Journal of Heat Transfer*, 1969. **91**(1): p. 100-104.
- Dawe, R.A. and Smith, E.B., Viscosity of Argon at High Temperatures. *Science*, 1969. **163**(3868): p. 675.
- Degroot, W.F. and Richards, G.N., Relative Rates of Carbon Gasification in Oxygen, Steam and Carbon-Dioxide. *Carbon*, 1989. **27**(2): p. 247-252.
- Devi, L., Ptasinski, K.J., and Janssen, F.J.J.G., A review of the primary measures for tar elimination in biomass gasification processes. *Biomass & Bioenergy*, 2003. **24**(2): p. 125-140.

- DiBlasi, C., Heat, momentum and mass transport through a shrinking biomass particle exposed to thermal radiation. *Chemical Engineering Science*, 1996. **51**(7): p. 1121-1132.
- Di Blasi, C., Modeling chemical and physical processes of wood and biomass pyrolysis. *Progress in Energy and Combustion Science*, 2008. **34**(1): p. 47-90.
- Di Blasi, C., Combustion and gasification rates of lignocellulosic chars. *Progress in Energy and Combustion Science*, 2009. **35**(2): p. 121-140.
- Diver, R.B., Miller, J.E., Allendorf, M.D., Siegel, N.P., and Hogan, R.E., Solar thermochemical water-splitting ferrite-cycle heat engines. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2008. **130**(4).
- Dupont, C., Boissonnet, G., Seller, J.M., Gauthier, P., and Schweich, D., Study about the kinetic processes of biomass steam gasification. *Fuel*, 2007. **86**(1-2): p. 32-40.
- Farmer, J.T. and Howell, J.R., Monte-Carlo Prediction of Radiative Heat-Transfer in Inhomogeneous, Anisotropic, Nongray Media. *Journal of Thermophysics and Heat Transfer*, 1994. 8(1): p. 133-139.
- Fiveland, W.A., Discrete Ordinate Methods for Radiative Heat-Transfer in Isotropically and Anisotropically Scattering Media. *Journal of Heat Transfer-Transactions of the Asme*, 1987. 109(3): p. 809-812.
- Fletcher, E.A. and Moen, R.L., Hydrogen and Oxygen from Water. *Science*, 1977. **197**(4308): p. 1050-1056.
- Fletcher, E.A., Solarthermal processing: A review. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2001. **123**(2): p. 63-74.
- Fogler, H.S., *Elements of Chemical Reaction Engineering*. 3 ed. 1999, Upper Saddle River, New Jersey: Prentice Hall.
- Francis, T.M., Lichty, P.R., and Weimer, A.W., Manganese oxide dissociation kinetics for the Mn2O3 thermochemical water-splitting cycle. Part 1: Experimental. *Chemical Engineering Science*, 2010. 65(12): p. 3709-3717.
- Fuller, E.N., Schettle.Pd, and Giddings, J.C., A New Method for Prediction of Binary Gas-Phase Diffusion Coefficients. *Industrial and Engineering Chemistry*, 1966. 58(5): p. 19.
- Funk, J.E. and Reinstro.Rm, Energy Requirements in Production of Hydrogen from Water. Industrial & Engineering Chemistry Process Design and Development, 1966. 5(3): p. 336.
- Funk, J.E., Thermochemical Processes for Production of Hydrogen from Water. *Abstracts of Papers of the American Chemical Society*, 1976: p. 21.

- Fushimi, C., Araki, K., Yamaguchi, Y., and Tsutsumi, A., Effect of heating rate on steam gasification of biomass. 1. Reactivity of char. *Industrial & Engineering Chemistry Research*, 2003. 42(17): p. 3922-3928.
- Gregg, D.W., Aiman, W.R., Otsuki, H.H., and Thorsness, C.B., Solar Coal-Gasification. *Solar Energy*, 1980. 24(3): p. 313-321.
- Gregg, D.W., Taylor, R.W., Campbell, J.H., Taylor, J.R., and Cotton, A., Solar Gasification of Coal, Activated Carbon, Coke and Coal and Biomass Mixtures. *Solar Energy*, 1980. 25(4): p. 353-364.
- Gronli, M.G. and Melaaen, M.C., Mathematical model for wood pyrolysis Comparison of experimental measurements with model predictions. *Energy & Fuels*, 2000. **14**(4): p. 791-800.
- Han, J. and Kim, H., The reduction and control technology of tar during biomass gasification/pyrolysis: An overview. *Renewable & Sustainable Energy Reviews*, 2008. 12(2): p. 397-416.
- Harris, D.J. and Smith, I.W., Intrinsic Reactivity of Coke and Char to Carbon-Dioxide. *Abstracts of Papers of the American Chemical Society*, 1989. **197**: p. 44.
- Haussener, S., Hirsch, D., Perkins, C., Weimer, A., Lewandowski, A., and Steinfeld, A., Modeling of a Multitube High-Temperature Solar Thermochemical Reactor for Hydrogen Production. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2009. 131(2).
- Haynes, W.M., ed. *CRC Handbook of Chemistry and Physics*. 91st ed. 2010, CRC Press / Taylor and Francis: Boca Raton, FL.
- Hermann, W.A., Quantifying global exergy resources. *Energy*, 2006. **31**(12): p. 1685-1702.
- Hinds, W.C., Aerosol Technology. 1982, New York: John Wiley and Sons.
- Hirsch, D. and Steinfeld, A., Radiative transfer in a solar chemical reactor for the co-production of hydrogen and carbon by thermal decomposition of methane. *Chemical Engineering Science*, 2004. **59**(24): p. 5771-5778.
- Hirsch, D. and Steinfeld, A., Solar hydrogen production by thermal decomposition of natural gas using a vortex-flow reactor. *International Journal of Hydrogen Energy*, 2004. **29**(1): p. 47-55.
- House, L.L. and Avery, L.W., Monte Carlo Technique Applied to Radiative Transfer. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1969. **9**(12): p. 1579.
- Howell, J.R. and Perlmutter, M., Monte-Carlo Solution of Radiant Heat Transfer in a Nongrey Nonisothermal Gas with Temperature Dependent Properties. *Aiche Journal*, 1964. **10**(4): p. 562-567.

- Howell, J.R. and Durkee, R.E., Radiative Transfer between Surfaces in a Cavity with Collimated Incident Radiation - Comparison of Analysis and Experiment. *Journal of Heat Transfer*, 1971. 93(2): p. 129.
- Howell, J.R., The Monte Carlo method in radiative heat transfer. *Journal of Heat Transfer-Transactions of the Asme*, 1998. **120**(3): p. 547-560.
- Incropera, F.P. and Dewitt, D.P., *Fundamentals of Heat and Mass Transfer*. 5th ed. 2002, New York: John Wiley and Sons.
- Ishii, M. and Mishima, K., 2-Fluid Model and Hydrodynamic Constitutive Relations. *Nuclear Engineering and Design*, 1984. **82**(2-3): p. 107-126.
- Ishii, M. and Hibiki, T., Thermo-Fluid Dynamics of Two-Phase Flow. 2006, New York: Springer Science-Business Media.
- Jansen, E., Overpeck, J., Briffa, K.R., Duplessy, J., Joos, F., Masson-Delmotte, V., Olago, D., Otto-Bliesner, B., Peltier, W.R., Rahmstorf, S., Ramesh, R., Raynaud, D., Rind, D., Solomina, O., Villalba, R., and Zhang, D., *Palaeoclimate*, in *Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change*, S. Soloman, D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Avery, M. Tignor, and H.L. Miller, Editors. 2007, Cambridge University Press: Cambridge.
- Johnson, J.L., Relationships between Coal-Char Gasification Reactivities and Physical and Chemical Coal and Coal-Char Properties. Abstracts of Papers of the American Chemical Society, 1975. 170(Aug24): p. 30.
- Joseph, J.H., Wiscombe, W.J., and Weinman, J.A., Delta-Eddington Approximation for Radiative Flux-Transfer. *Journal of the Atmospheric Sciences*, 1976. **33**(12): p. 2452-2459.
- Juntgen, H., Reactivities of Carbon to Steam and Hydrogen and Applications to Technical Gasification Processes a Review. *Carbon*, 1981. **19**(3): p. 167-173.
- Keunecke, M., Meier, A., and Palumbo, R., Solar thermal decomposition of zinc oxide: an initial investigation of the recombination reaction in the temperature range 1100-1250K. *Chemical Engineering Science*, 2004. **59**(13): p. 2695-2704.
- Klein, H.H., Karni, J., Ben-Zvi, R., and Bertocchi, R., Heat transfer in a directly irradiated solar receiver/reactor for solid-gas reactions. *Solar Energy*, 2007. **81**(10): p. 1227-1239.
- Klose, W. and Wolki, M., On the intrinsic reaction rate of biomass char gasification with carbon dioxide and steam. *Fuel*, 2005. **84**(7-8): p. 885-892.
- Kodama, T., High-temperature solar chemistry for converting solar heat to chemical fuels. *Progress in Energy and Combustion Science*, 2003. **29**(6): p. 567-597.

- Kodama, T., Kondoh, Y., Yamamoto, R., Andou, H., and Satou, N., Thermochemical hydrogen production by a redox system of ZrO2-supported Co(II)-ferrite. *Solar Energy*, 2005. 78(5): p. 623-631.
- Kodama, T. and Gokon, N., Thermochernical cycles for high-temperature solar hydrogen production. *Chemical Reviews*, 2007. **107**(10): p. 4048-4077.
- Kogan, A., Direct solar thermal splitting of water and on-site separation of the products II. Experimental feasibility study. *International Journal of Hydrogen Energy*, 1998. **23**(2): p. 89-98.
- Kogan, A., Spiegler, E., and Wolfshtein, M., Direct solar thermal splitting of water and on-site separation of the products. III. Improvement of reactor efficiency by steam entrainment. *International Journal of Hydrogen Energy*, 2000. 25(8): p. 739-745.
- Kogan, A., Direct solar thermal splitting of water and on-site separation of the products IV. Development of porous ceramic membranes for a solar thermal water-splitting reactor. *International Journal of Hydrogen Energy*, 2000. **25**(11): p. 1043-1050.
- Kogan, M. and Kogan, A., Production of hydrogen and carbon by solar thermal methane splitting. I. The unseeded reactor. *International Journal of Hydrogen Energy*, 2003. 28(11): p. 1187-1198.
- Kogan, A., Israeli, M., and Alcobi, E., Production of hydrogen and carbon by solar thermal methane splitting. IV. Preliminary simulation of a confined tornado flow configuration by computational fluid dynamics. *International Journal of Hydrogen Energy*, 2007. **32**(18): p. 4800-4810.
- Kolb, G. and Diver, R.B., *Screening Analysis of Solar Thermochemical Hydrogen Concepts*. 2008, Sandia National Laboratories: Albuquerque, New Mexico.
- Koo, H.M., Vaillon, R., Goutiere, V., Le Dez, V., Cha, H., and Song, T.H., Comparison of three discrete ordinates methods applied to two-dimensional curved geometries. *International Journal of Thermal Sciences*, 2003. 42(4): p. 343-359.
- Lathrop, K.D., Ray Effects in Discrete Ordinates Equations. *Nuclear Science and Engineering*, 1968. **32**(3): p. 357.
- Laurendeau, N.M., Heterogeneous Kinetics of Coal Char Gasification and Combustion. *Progress in Energy and Combustion Science*, 1978. **4**(4): p. 221-270.
- Lede, J., Solar thermochemical conversion of biomass. Solar Energy, 1999. 65(1): p. 3-13.
- Lewandowski, A., Bingham, C., Ogallagher, J., Winston, R., and Sagie, D., Performance Characterization of the Seri High-Flux Solar Furnace. *Solar Energy Materials*, 1991. 24(1-4): p. 550-563.

- Li, H.S., Flamant, G., and Lu, J.D., Mitigation of ray effects in the discrete ordinates method. *Numerical Heat Transfer Part B-Fundamentals*, 2003. **43**(5): p. 445-466.
- Li, H.S. and Werther, J., Computation of radiative image formation in isolated source and collimated irradiation problems. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2006. **97**(1): p. 142-159.
- Lichty, P., Perkins, C., Woodruff, B., Bingham, C., and Weimer, A., Rapid High Temperature Solar Thermal Biomass Gasification in a Prototype Cavity Reactor. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(1).
- Linstrom, P.J., and Mallard, W.G., NIST Chemistry WebBook, NIST Standard Reference Database Number 69, National Institute of Standards and Technology, Gaithersburg MD, 20899, <u>http://webbook.nist.gov.</u>, ed.
- Lipinski, W., Z'Graggen, A., and Steinfeld, A., Transient radiation heat transfer within a nongray nonisothermal absorbing-emitting-scattering suspension of reacting particles undergoing shrinkage. *Numerical Heat Transfer Part B-Fundamentals*, 2005. 47(5): p. 443-457.
- Lipinski, W., Thommen, D., and Steinfeld, A., Unsteady radiative heat transfer within a suspension of ZnO particles undergoing thermal dissociation. *Chemical Engineering Science*, 2006. 61(21): p. 7029-7035.
- Long, F.J. and Sykes, K.W., The Mechanism of the Steam-Carbon Reaction. Proceedings of the Royal Society of London Series a-Mathematical and Physical Sciences, 1948. 193(1034): p. 377-399.
- Maag, G., Lipinski, W., and Steinfeld, A., Particle-gas reacting flow under concentrated solar irradiation. *International Journal of Heat and Mass Transfer*, 2009. **52**(21-22): p. 4997-5004.
- Maag, G. and Steinfeld, A., Design of a 10 MW Particle-Flow Reactor for Syngas Production by Steam-Gasification of Carbonaceous Feedstock Using Concentrated Solar Energy & *Fuels*, 2010. **24**: p. 6540-6547.
- Maag, G., Rodat, S., Flamant, G., and Steinfeld, A., Heat transfer model and scale-up of an entrained-flow solar reactor for the thermal decomposition of methane. *International Journal of Hydrogen Energy*, 2010. **35**(24): p. 13232-13241.
- Maltby, J.D. and Burns, P.J., Performance, Accuracy, and Convergence in a 3-Dimensional Monte-Carlo Radiative Heat-Transfer Simulation. *Numerical Heat Transfer Part B-Fundamentals*, 1991. 19(2): p. 191-209.
- Mann, M.D., Knutson, R.Z., Erjavec, J., and Jacobsen, J.P., Modeling reaction kinetics of steam gasification for a transport gasifier. *Fuel*, 2004. **83**(11-12): p. 1643-1650.
- Manovic, V., Komatina, M., and Oka, S., Modeling the temperature in coal char particle during fluidized bed combustion. *Fuel*, 2008. **87**(6): p. 905-914.

- Marban, G. and Vales-Solis, T., Towards the hydrogen economy? *International Journal of Hydrogen Energy*, 2007. **32**(12): p. 1625-1637.
- Martinek, J., Channel, M., Lewandowski, A., and Weimer, A.W., Considerations for the Design of Solar-Thermal Chemical Processes. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(3).
- Mayers, M.A., The rate of oxidation of graphite by steam. *Journal of the American Chemical Society*, 1934. **56**(7): p. 1879-1881.
- Meier, A., Ganz, J., and Steinfeld, A., Modeling of a novel high-temperature solar chemical reactor. *Chemical Engineering Science*, 1996. **51**(11): p. 3181-3186.
- Meier, A., Bonaldi, E., Cella, G.M., Lipinski, W., Wuillemin, D., and Palumbo, R., Design and experimental investigation of a horizontal rotary reactor for the solar thermal production of lime. *Energy*, 2004. 29(5-6): p. 811-821.
- Melchior, T., Perkins, C., Weimer, A.W., and Steinfeld, A., A cavity-receiver containing a tubular absorber for high-temperature thermochemical processing using concentrated solar energy. *International Journal of Thermal Sciences*, 2008. 47(11): p. 1496-1503.
- Melchior, T. and Steinfeld, A., Radiative transfer within a cylindrical cavity with diffusely/specularly reflecting inner walls containing an array of tubular absorbers. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2008. **130**(2).
- Melchior, T., Perkins, C., Lichty, P., Weimer, A.W., and Steinfeld, A., Solar-driven biochar gasification in a particle-flow reactor. *Chemical Engineering and Processing*, 2009. 48(8): p. 1279-1287.
- Miller, R.S. and Bellan, J., A generalized biomass pyrolysis model based on superimposed cellulose, hemicellulose and lignin kinetics. *Combustion Science and Technology*, 1997. 126(1-6): p. 97-137.
- Modest, M.F., Three-Dimensional Radiative Exchnag Factors for Nongray Nondiffuse Surfaces. *Numerical Heat Transfer Part B-Fundamentals*, 1978. **1**(3): p. 403-416.
- Moller, S. and Palumbo, R., The development of a solar chemical reactor for the direct thermal dissociation of zinc oxide. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2001. **123**(2): p. 83-90.
- Montgomery, D., *Design and Analysis of Experiments*. 6th ed. 2005, New York: John Wiley and Sons.
- Muhlen, H.J., Vanheek, K.H., and Juntgen, H., Kinetic-Studies of Steam Gasification of Char in the Presence of H-2, Co2 and Co. *Fuel*, 1985. **64**(7): p. 944-949.

- Muller, R., Von Zedtwitz, P., Wokaun, A., and Steinfeld, A., Kinetic investigation on steam gasification of charcoal under direct high-flux irradiation. *Chemical Engineering Science*, 2003. 58(22): p. 5111-5119.
- Muller, R., Lipinski, W., and Steinfeld, A., Transient heat transfer in a directly-irradiated solar chemical reactor for the thermal dissociation of ZnO. *Applied Thermal Engineering*, 2008. 28(5-6): p. 524-531.
- Murthy, J.Y. and Mathur, S.R., Finite volume method for radiative heat transfer using unstructured meshes. *Journal of Thermophysics and Heat Transfer*, 1998. **12**(3): p. 313-321.
- Nakamura, T., Hydrogen Production from Water Utilizing Solar Heat at High-Temperatures. *Solar Energy*, 1977. **19**(5): p. 467-475.
- Otto, K., Bartosiewicz, L., and Shelef, M., Catalytic Steam Gasification of Graphite Effects of Calcium, Strontium, and Barium with and without Sulfur. *Carbon*, 1979. **17**(4): p. 351-357.
- Ozalp, N. and Kanjirakat, A., A Computational Fluid Dynamics Study on the Effect of Carbon Particle Seeding for the Improvement of Solar Reactor Performance. *Journal of Heat Transfer-Transactions of the Asme*, 2010. **132**(12).
- Palik, E.D., ed. Handbook of Optical Constants of Solids. 1998, Academic Press: San Diego.
- Palumbo, R., Lede, J., Boutin, O., Ricart, E.E., Steinfeld, A., Moller, S., Weidenkaff, A., Fletcher, E.A., and Bielicki, J., The production of Zn from ZnO in a high-temperature solar decomposition quench process - I. The scientific framework for the process. *Chemical Engineering Science*, 1998. 53(14): p. 2503-2517.
- Palumbo, R., Keunecke, M., Moller, S., and Steinfeld, A., Reflections on the design of solar thermal chemical reactors: thoughts in transformation. *Energy*, 2004. **29**(5-6): p. 727-744.
- Pangborn, J.K. and Sharer, J.C., Analysis of Thermochemical Water-Splitting Cycles, in Proceedings of the Hydrogen Economy Miami Energy Conference (THEME), T.N. Veziroglu, Editor. 1975, Plenum Press: Miami, FL. p. 499-515.
- Papadikis, K., Gu, S., and Bridgwater, A.V., CFD modelling of the fast pyrolysis of biomass in fluidised bed reactors. Part B Heat, momentum and mass transport in bubbling fluidised beds. *Chemical Engineering Science*, 2009. 64(5): p. 1036-1045.
- Perkins, C. and Weimer, A.W., Likely near-term solar-thermal water splitting technologies. *International Journal of Hydrogen Energy*, 2004. **29**(15): p. 1587-1599.
- Perkins, C., Lichty, P., Weimer, A.W., and Bingham, C., Fluid-wall effectiveness for preventing oxidation in solar-thermal ZnO reactors. *Aiche Journal*, 2007. **53**(7): p. 1830-1844.
- Perkins, C., Lichty, P.R., and Weimer, A.W., Thermal ZnO dissociation in a rapid aerosol reactor as part of a solar hydrogen production cycle. *International Journal of Hydrogen Energy*, 2008. **33**(2): p. 499-510.

- Perry, R.H. and Green, D.W., eds. *Perry's Chemical Engineers' Handbook*. 7th ed. 1997, McGraw-Hill: New York.
- Petrasch, J. and Steinfeld, A., Dynamics of a solar thermochemical reactor for steam-reforming of methane. *Chemical Engineering Science*, 2007. **62**(16): p. 4214-4228.
- Petrasch, J., Osch, P., and Steinfeld, A., Dynamics and control of solar thermochemical reactors. *Chemical Engineering Journal*, 2009. **145**(3): p. 362-370.
- Piatkowski, N., Wieckert, C., and Steinfeld, A., Experimental investigation of a packed-bed solar reactor for the steam-gasification of carbonaceous feedstocks. *Fuel Processing Technology*, 2009. **90**(3): p. 360-366.
- Poling, B.E., Prausnitz, J.M., and O'Connel, J.P., *The Properties of Gases and Liquids*. 5th ed. 2001, New York: McGraw-Hill.
- Pregger, T., Graf, D., Krewitt, W., Sattler, C., Roeb, M., and Moller, S., Prospects of solar thermal hydrogen production processes. *International Journal of Hydrogen Energy*, 2009. 34(10): p. 4256-4267.
- Prins, M.J., Ptasinski, K.J., and Janssen, F.J.J.G., From coal to biomass gasification: Comparison of thermodynamic efficiency. *Energy*, 2007. **32**(7): p. 1248-1259.
- Raithby, G.D. and Chui, E.H., A Finite-Volume Method for Predicting a Radiant-Heat Transfer in Enclosures with Participating Media. *Journal of Heat Transfer-Transactions of the Asme*, 1990. **112**(2): p. 415-423.
- Raithby, G.D., Evaluation of discretization errors in finite-volume radiant heat transfer predictions. *Numerical Heat Transfer Part B-Fundamentals*, 1999. **36**(3): p. 241-264.
- Roberts, D.G. and Harris, D.J., Char gasification with O-2, CO2, and H2O: Effects of pressure on intrinsic reaction kinetics. *Energy & Fuels*, 2000. 14(2): p. 483-489.
- Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., Hydrogen production from solar thermal dissociation of natural gas: development of a 10 kW solar chemical reactor prototype. *Solar Energy*, 2009. **83**(9): p. 1599-1610.
- Rodat, S., Abanades, S., Sans, J.L., and Flamant, G., A pilot-scale solar reactor for the production of hydrogen and carbon black from methane splitting. *International Journal of Hydrogen Energy*, 2010. **35**(15): p. 7748-7758.
- Roeb, M., Sattler, C., Kluser, R., Monnerie, N., de Oliveira, L., Konstandopoulos, A.G., Agrafiotis, C., Zaspalis, V.T., Nalbandian, L., Steele, A., and Stobbe, P., Solar hydrogen production by a two-step cycle based on mixed iron oxides. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2006. **128**(2): p. 125-133.

- Rosner, D.E. and Park, H.M., Thermophoretically Augmented Mass-Transfer Momentum-Transfer and Energy-Transfer Rates in High Particle Mass Loaded Laminar Forced-Convection Systems. *Chemical Engineering Science*, 1988. **43**(10): p. 2689-2704.
- Sakami, M. and Charette, A., Application of a modified discrete ordinates method to twodimensional enclosures of irregular geometry. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 2000. **64**(3): p. 275-298.
- Schaffner, B., Meier, A., Wuillemin, D., Hoffelner, W., and Steinfeld, A., Recycling of hazardous solid waste material using high-temperature solar process heat. 2. Reactor design and experimentation. *Environmental Science & Technology*, 2003. **37**(1): p. 165-170.
- Scheffe, J.R., Li, J.H., and Weimer, A.W., A spinel ferrite/hercynite water-splitting redox cycle. *International Journal of Hydrogen Energy*, 2010. **35**(8): p. 3333-3340.
- Schunk, L.O., Lipinski, W., and Steinfeld, A., Heat transfer model of a solar receiver-reactor for the thermal dissociation of ZnO-Experimental validation at 10 kW and scale-up to 1 MW. *Chemical Engineering Journal*, 2009. **150**(2-3): p. 502-508.
- Siegel, R. and Howell, J., *Thermal Radiation Heat Transfer*. 4 ed. 2002, New York: Taylor and Francis.
- Siegel, N.P., Ho, C.K., Khalsa, S.S., and Kolb, G.J., Development and Evaluation of a Prototype Solid Particle Receiver: On-Sun Testing and Model Validation. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2010. **132**(2).
- Singh, B.P. and Kaviany, M., Independent Theory Versus Direct Simulation of Radiation Heat-Transfer in Packed-Beds. *International Journal of Heat and Mass Transfer*, 1991. 34(11): p. 2869-2882.
- Singh, B.P. and Kaviany, M., Modeling Radiative Heat-Transfer in Packed-Beds. *International Journal of Heat and Mass Transfer*, 1992. **35**(6): p. 1397-1405.
- Smith, T.F., Shen, Z.F., and Friedman, J.N., Evaluation of Coefficients for the Weighted Sum of Gray Gases Model. *Journal of Heat Transfer-Transactions of the Asme*, 1982. **104**(4): p. 602-608.
- Steinfeld, A. and Fletcher, E.A., A Solar Receiver-Reactor with Specularly Reflecting Walls for High-Temperature Thermoelectrochemical and Thermochemical Processes. *Energy*, 1988. 13(4): p. 301-311.
- Steinfeld, A. and Schubnell, M., Optimum Aperture Size and Operating Temperature of a Solar Cavity-Receiver. Solar Energy, 1993. 50(1): p. 19-25.
- Steinfeld, A., Larson, C., Palumbo, R., and Foley, M., Thermodynamic analysis of the coproduction of zinc and synthesis gas using solar process heat. *Energy*, 1996. **21**(3): p. 205-222.

- Steinfeld, A. and Spiewak, I., Economic evaluation of the solar thermal CO-production of zinc and synthesis gas. *Energy Conversion and Management*, 1998. **39**(15): p. 1513-1518.
- Steinfeld, A., Solar hydrogen production via a two-step water-splitting thermochemical cycle based on Zn/ZnO redox reactions. *International Journal of Hydrogen Energy*, 2002. 27(6): p. 611-619.
- Steinfeld, A., Solar thermochemical production of hydrogen a review. *Solar Energy*, 2005. **78**(5): p. 603-615.
- Steinfeld, A. and Weimer, A.W., Thermochemical Production of Fuels with Concentrated Solar Energy. Optics Express, 2010. 18(9): p. A100-A111.
- Stratmann, F., Otto, E., and Fissan, H., Thermophoretical and Diffusional Particle-Transport in Cooled Laminar Tube Flow. *Journal of Aerosol Science*, 1994. 25(7): p. 1305-1319.
- Sturzenegger, M., Ganz, J., Nuesch, P., and Schelling, T., Solar hydrogen from a manganese oxide based thermochemical cycle. *Journal De Physique Iv*, 1999. **9**(P3): p. 331-335.
- Sturzenegger, M. and Nuesch, P., Efficiency analysis for a manganese-oxide-based thermochemical cycle. *Energy*, 1999. **24**(11): p. 959-970.
- Sudiro, M., Pellizzaro, M., Bezzo, F., and Bertucco, A., Simulated moving bed technology applied to coal gasification. *Chemical Engineering Research & Design*, 2010. **88**(4A): p. 465-475.
- Surzhikov, S.T. and Howell, J.R., Monte Carlo simulation of radiation in scattering volumes with line structure. *Journal of Thermophysics and Heat Transfer*, 1998. **12**(2): p. 278-281.
- Szargut, J., Chemical Exergies of the Elements. Applied Energy, 1989. 32(4): p. 269-286.
- Tamaura, Y., Steinfeld, A., Kuhn, P., and Ehrensberger, K., Production of Solar Hydrogen by a Novel, 2-Step, Water-Splitting Thermochemical Cycle. *Energy*, 1995. 20(4): p. 325-330.
- Tan, H.P., Zhang, H.C., and Zhen, B., Estimation of ray effect and false scattering in approximate solution method for thermal radiative transfer equation. *Numerical Heat Transfer Part a-Applications*, 2004. **46**(8): p. 807-829.
- Taniguchi, H., Kudo, K., Otaka, M., Sumarsono, M., and Obata, M., Development of a Monte-Carlo Method for Numerical-Analysis on Radiative Energy-Transfer through Nongrey-Gas Layer. *International Journal for Numerical Methods in Engineering*, 1992. 35(4): p. 883-891.
- Taylor, R.W., Berjoan, R., and Coutures, J.P., Solar Gasification of Carbonaceous Materials. Solar Energy, 1983. 30(6): p. 513-525.
- Tescari, S., Mazet, N., and Neveu, P., Constructal method to optimize solar thermochemical reactor design. *Solar Energy*, 2010. **84**(9): p. 1555-1566.

- Tescari, S., Mazet, N., Neveu, P., and Abanades, S., Optimization Model for Solar Thermochemical Reactor: Efficiency Increase by a Nonuniform Heat Sink Distribution. *Journal of Solar Energy Engineering-Transactions of the Asme*, 2011. **133**(3).
- Tewari, Y.B. and Goldberg, R.N., Thermodynamics of Hydrolysis of Disaccharides Cellobiose, Gentiobiose, Isomaltose, and Maltose. *Journal of Biological Chemistry*, 1989. **264**(7): p. 3966-3971.
- Toor, J.S. and Viskanta, R., A Numerical Experiment of Radiant Heat Interchange by Monte Carlo Method. *International Journal of Heat and Mass Transfer*, 1968. **11**(5): p. 883.
- Touloukain, Y.S. and DeWitt, D.P., *Thermophysical Properties of Matter the TPRC Data Series*. Thermal radiative properties: metallic elements and alloys. Vol. 7. 1970, New York: Plenum Publishing.
- Trenberth, K.E., Jones, P.D., Ambenje, P., Bojariu, R., Easterling, D., Klein Tank, A., Parker, D., Rahimzadeh, F., Renwick, J.A., Rusticucci, M., Soden, B., and Zhai, P., Observations: Surface and Atmospheric Climate Change, in Climate Change 2007: The Physical Science Basis. Contribution of Working Group I to the Fourth Assessment Report of the Intergovernmental Panel on Climate Change, S. Soloman, D. Qin, M. Manning, Z. Chen, M. Marquis, K.B. Avery, M. Tignor, and H.L. Miller, Editors. 2007, Cambridge University Press: Cambridge.
- Trommer, D., Noembrini, F., Fasciana, A., Rodriguez, D., Morales, A., Romero, M., and Steinfeld, A., Hydrogen production by steam-gasification of petroleum coke using concentrated solar power - I. Thermodynamic and kinetic analyses. *International Journal of Hydrogen Energy*, 2005. **30**(6): p. 605-618.
- Trommer, D. and Steinfeld, A., Kinetic modeling for the combined pyrolysis and steam gasification of petroleum coke and experimental determination of the rate constants by dynamic thermogravimetry in the 500-1520 K range. *Energy & Fuels*, 2006. **20**(3): p. 1250-1258.
- Trommer, D., Thermodynamic and Kinetic Analyses of the Solar Thermal Gasification of Petroleum Coke. 2006, Swiss Federal Institute of Technology: Zurich.
- Truelove, J.S., 3-Dimensional Radiation in Absorbing Emitting Scattering Media Using the Discrete-Ordinates Approximation. *Journal of Quantitative Spectroscopy & Radiative Transfer*, 1988. **39**(1): p. 27-31.
- Versteeg, H.K. and Malalasekera, W., *An Introduction to Computational Fluid Dynamics*. 2nd ed. 2007, Harlow, England: Pearson Education.
- von Zedtwitz, P. and Steinfeld, A., Steam-gasification of coal in a fluidized-bed/packed-bed reactor exposed to concentrated thermal radiation-modeling and experimental validation. *Industrial & Engineering Chemistry Research*, 2005. **44**(11): p. 3852-3861.

- von Zedtwitz, P., Lipinski, W., and Steinfeld, A., Numerical and experimental study of gasparticle radiative heat exchange in a fluidized-bed reactor for steam-gasification of coal. *Chemical Engineering Science*, 2007. **62**(1-2): p. 599-607.
- Walker, P.L., Foresti, R.J., and Wright, C.C., Surface Area Studies of Carbon-Carbon Dioxide Reaction. *Industrial and Engineering Chemistry*, 1953. 45(8): p. 1703-1710.
- Walsh, J.K., Weimer, A.W., and Hrenya, C.M., Thermophoretic deposition of aerosol particles in laminar tube flow with mixed convection. *Journal of Aerosol Science*, 2006. **37**(6): p. 715-734
- Wang, Y. and Kinoshita, C.M., Kinetic-Model of Biomass Gasification. *Solar Energy*, 1993. **51**(1): p. 19-25.
- Watanabe, H. and Otaka, M., Numerical simulation of coal gasification in entrained flow coal gasifier. *Fuel*, 2006. **85**(12-13): p. 1935-1943.
- Weimer, A.W. and Clough, D.E., Modeling of Char Particle Size-Conversion Distributions in a Fluidized-Bed Gasifier - Non-Isothermal Effects. *Powder Technology*, 1980. 27(1): p. 85-103.
- Wendelin, T. SolTRACE: A new optical modeling tool for concentrating solar optics. in Proceedings of the ISEC: International Solar Energy Conference. 2003. Kohala Coast, Hawaii: American Society of Mechanical Engineers.
- Wiebelt, J.A and Ruo, S.Y., Radiant-interchange configuration factors for finite right circular cylinder to rectangular plane. *International Journal of Heat and Mass Transfer*, 1963. 6(2): p. 143-146.
- Wieckert, C., Palumbo, R., and Frommherz, U., A two-cavity reactor for solar chemical processes: heat transfer model and application to carbothermic reduction of ZnO. *Energy*, 2004. 29(5-6): p. 771-787.
- Yang, Y.S., Howell, J.R., and Klein, D.E., Radiative Heat-Transfer through a Randomly Packed-Bed of Spheres by the Monte-Carlo Method. *Journal of Heat Transfer-Transactions of the Asme*, 1983. 105(2): p. 325-332.
- Yarbrough, D. and C., L., Monte Carlo Calculation of Radiation View Factors, in Integral Methods in Science and Engineering, F. Payne, Editor. 1986, Hemisphere: Washington, DC. p. 563-574.
- Yu, Q.Z., Brage, C., Chen, G.X., and Sjostrom, K., Temperature impact on the formation of tar from biomass pyrolysis in a free-fall reactor. *Journal of Analytical and Applied Pyrolysis*, 1997. 40-1: p. 481-489.
- Z'Graggen, A., Haueter, P., Trommer, D., Romero, M., de Jesus, J.C., and Steinfeld, A., Hydrogen production by steam-gasification of petroleum coke using concentrated solar

power - II - Reactor design, testing, and modeling. *International Journal of Hydrogen Energy*, 2006. **31**(6): p. 797-811.

- Z'Graggen, A. and Steinfeld, A., Hydrogen production by steam-gasification of carbonaceous materials using concentrated solar energy V. Reactor modeling, optimization, and scale-up. *International Journal of Hydrogen Energy*, 2008. **33**(20): p. 5484-5492.
- Z'Graggen, A. and Steinfeld, A., A two-phase reactor model for the steam-gasification of carbonaceous materials under concentrated thermal radiation. *Chemical Engineering and Processing*, 2008. **47**(4): p. 655-662.
- Z'Graggen, A. and Steinfeld, A., Heat and mass transfer analysis of a suspension of reacting particles subjected to concentrated solar radiation Application to the steam-gasification of carbonaceous materials. *International Journal of Heat and Mass Transfer*, 2009. **52**(1-2): p. 385-395.

## **Appendix A**:

### Characteristic times and dimensionless parameters

#### A.1 Characteristic times

Characteristic times associated with external heat transfer processes are determined from a macroscopic energy balance on the particle under the assumption of uniform internal particle temperature. The macroscopic energy balance including both convective heat transfer with the fluid phase and radiative exchange with the tube walls is given by equation A.1 in which  $A_p$  is the surface area of the particle, h is the heat transfer coefficient with the surrounding fluid phase,  $m_p$ ,  $C_p$  and  $\varepsilon_p$  are, respectively, the particle mass, heat capacity, and surface emissivity,  $T_p$  is the particle temperature,  $T_g$  is the temperature of the surrounding fluid and  $T_w$  is the tube wall temperature.

$$\frac{d(m_p C_p T_p)}{dt} = A_p h \left( T_g - T_p \right) + A_p \varepsilon_p \sigma \left( T_w^4 - T_p^4 \right) \tag{A.1}$$

Analytical solutions to equation A.1 can be derived with external heat transfer accomplished either exclusively by convection or exclusively by radiation. Assuming an initial particle temperature of  $T_{p0}$ , and neglecting radiation heat transfer, the analytical solution of equation A.1 is given by equation A.2.

$$\frac{T_{p} - T_{p0}}{T_{g} - T_{p0}} = 1 - \exp\left(-\frac{A_{p}h}{m_{p}C_{p}}t\right)$$
(A.2)

The analytical solution of equation A.1 neglecting convective heat transfer is shown in equation A.3 with initial particle temperature  $T_{p0}$  [1].

$$t = \frac{m_p C_p}{2T_w^3 A_p \varepsilon_p \sigma} \left\{ \frac{1}{2} \ln \left[ \left( \frac{T_w + T_p}{T_w + T_{p0}} \right) \left( \frac{T_w - T_{p0}}{T_w - T_p} \right) \right] + \tan^{-1} \left( \frac{(T_p - T_{p0})/T_w}{1 + (T_p T_{p0})/T_w} \right) \right\}$$
(A.3)

The characteristic time for external convection/conduction heat transfer is defined as the time at which

$$\frac{T_p - T_{p0}}{T_g - T_{p0}} \text{ or } \frac{T_p - T_{p0}}{T_w - T_{p0}} = 1 - e^{-1} = 0.632$$
(A.4)

The characteristic time for external convection based on this definition is given by equation A.5 where  $d_p$  is the particle diameter,  $\rho_p$  is the particle density,  $k_g$  is the thermal conductivity of the gas phase, and the convection coefficient has been evaluated under conditions at which there is a negligible slip velocity between fluid and particulate phases.

$$t_{c,conv} = \frac{m_p C_p}{A_p h} = \frac{\rho_p C_p d_p^2}{12k_g}$$
(A.5)

Following the definition in eqn. *A.4*, the characteristic time for external radiative heat transfer is given in equation A.6 [1].

$$t_{c,rad} = \frac{\rho_p C_p d_p}{24T_w^3 \varepsilon_p \sigma} f(T_{p0}/T_w) \approx \frac{\rho_p C_p d_p}{24T_w^3 \varepsilon_p \sigma}$$
(A.6)

$$f(T_{p0}/T_{w}) = \left\{ \ln\left[\frac{1.632 - 1.264(T_{p0}/T_{w}) - 0.368(T_{p0}/T_{w})^{2}}{0.368[1 - (T_{p0}/T_{w})^{2}]}\right] + 2\tan^{-1}\left(\frac{0.632[1 - (T_{p0}/T_{w})]}{1.632 + 0.632(T_{p0}/T_{w}) + 0.368(T_{p0}/T_{w})^{2}}\right)\right\} \quad (A.7)$$

The function  $f(T_{p0}/T_w)$  varies weakly over realistic particle and wall temperatures with 2.62 >  $f(T_{p0}/T_w) > 1$  over  $0 < T_{p0}/T_w < 1$  and is typically ignored in calculations of  $t_{c,rad}$ .

Transient internal heat conduction within the particle is described by the partial differential equation in equation A.8 where  $\alpha$  is the thermal diffusivity of the particle, *R* is the particle radius,  $T_{\infty}$  is the fixed external particle surface temperature, and  $T_0$  is the initial particle temperature.
$$\frac{\partial T_p}{\partial t} = \frac{\alpha}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) \qquad \begin{array}{l} t = 0 : T_p = T_0 \\ r = R : T_p = T_{\infty} \end{array}$$
(A.8)

The analytical solution to eqn. A.8 at the center of the particle (r = 0) is given by equation A.9.

$$\frac{T_p - T_{p0}}{T_{\infty} - T_{p0}} = 1 - 2\sum_{n=1}^{\infty} (-1)^{n+1} \exp\left(\frac{-n^2 \pi^2 \alpha}{R^2}t\right)$$
(A.9)

For  $\alpha t/R^2$  greater than 0.15 the infinite sum can be reasonably approximated by a single term. The characteristic time for internal conduction is defined analogously to that for external convection in equation A.10 and given approximately by equation A.11 in which  $k_p$  is the thermal conductivity of the particle material.

$$\frac{T_p(r=0) - T_{p0}}{T_{\infty} - T_{p0}} = 0.632 \tag{A.10}$$

$$t_{c,cond\_int} \approx \frac{\rho_p C_p d_p^2}{24k_p} \tag{A.11}$$

Figures A.1 and A.2 show the calculated characteristic times for carbon particles entrained in argon gas for two ranges of particle diameter. For nanometer-sized particles the characteristic times associated with convection and internal conduction are several orders of magnitude smaller than that associated with external radiation heat transfer between the wall and the particles implying that particle and local gas phase temperatures equilibrate rapidly once the particles are heated by radiation thereby justifying the assumption of uniform internal particle temperature and equivalent local particle and gas phase temperatures. Figure A.2 shows that this assumption does not begin to break down until the particle diameter exceeds roughly 20  $\mu$ m. Thus the presence of particle aggregates will not limit the validity of the model assumptions until aggregates reach approximately 500 times the diameter of the individual particles.



Figure A.1: Ratios of characteristic times for  $d_p < 100$  nm



Figure A.2: Ratios of characteristic times for  $d_p < 50 \ \mu m$ 

# A.2 Dimensionless parameters

The momentum and thermal Stokes numbers are given in equations A.12 and A.13 [2-5].

$$St = \frac{\tau_p}{\tau_{flow}} = \frac{\rho_p d_p^2 C_c}{18\mu} \frac{\nu}{L}$$
(A.12)

$$St = \frac{\tau_{p,th}}{\tau_{flow}} = \frac{\rho_p d_p^2 C p_p}{12k_g} \frac{\upsilon}{L}$$
(A.13)

The largest value of the Stokes number occurs at the tube centerline where the fluid velocity is maximized. Figures A.3 and A.4 show the momentum and thermal Stokes numbers as a function of particle diameter, temperature, and total fluid flow rate with fluid velocity taken to be the maximum velocity from a fully developed laminar flow profile at temperature T.



Figure A.3: Momentum Stokes number for  $d_p < 40 \ \mu m$ 



Figure A.4: Thermal Stokes number for  $d_p < 40 \ \mu m$ 

The momentum and thermal Stokes numbers for the nominal 42 nm particle diameter considered in this study are on the order of  $10^{-7} - 10^{-5}$  and thus the assumptions of equivalent fluid and particle phase temperatures and velocities are clearly valid. Figures A.3 and A.4 show that the assumptions controlled by low momentum and thermal Stokes numbers appear to break down for a particle diameter on the order of 5-30  $\mu$ m depending on fluid flow rate.

For a momentum Stokes number well under unity the velocity discrepancy between the fluid and particulate phases is negligible, leading to a Biot number given by equation A.14 based on external convective transport with Nu = 2 [6].

$$Bi = \frac{hd_p}{k_p} = Nu \frac{k_g}{k_p}$$
(A.14)

The Biot number based on external radiative exchange with tube walls in the absence of convection can be derived as shown in equation A.15 and is similar to that defined by both Maag and Lipinski [7, 8].

$$Bi_{r} = \frac{d_{p}}{k_{p}} \left\{ \frac{\sigma \left(T_{w}^{2} + T_{p}^{2}\right) \left(T_{w} + T_{p}\right)}{\frac{1}{\varepsilon_{p}} + F_{w-p} \left(\frac{1}{\varepsilon_{w}} - 1\right)} \right\} \approx \frac{d_{p}}{k_{p}} \varepsilon_{p} \sigma \left(T_{w}^{2} + T_{p}^{2}\right) \left(T_{w} + T_{p}\right)$$
(A.15)

Both convective and radiative Biot numbers are shown in Figure A.5 as a function of particle temperature and diameter. The wall temperature for  $Bi_r$  is maintained at a constant value of 1800 K. With negligible slip velocity the convective Biot number is independent of particle diameter whereas the radiative Biot number increases strongly with particle diameter. Figure A.5 reveals that the assumption of uniform internal particle temperature appears to be valid for all particle diameters less than 10  $\mu$ m for the conditions considered in this study.



Figure A.6 shows the effectiveness factor for the global surface reaction model detailed in Chapter 5 as a function of particle size and temperature with a solid porosity of 0.2 and the particle density, specific surface area, and reaction kinetic parameters discussed in Chapter 5. For spherical particles the effectiveness factor is given as a function of the Thiele modulus in equation A.16 [9].

$$\eta = \frac{3}{\phi} \left( \frac{1}{\tanh \phi} - \frac{1}{\phi} \right) \tag{A.16}$$



Figure A.6: Effectiveness factor for  $d_p < 30 \ \mu m$ 

The effectiveness factor is greater than 0.9 for a particle diameter up to 5  $\mu$ m even at T = 2000 K.

Figures A.1-A.6 indicate that the assumptions of equivalent fluid and particulate phase temperature and velocity, as well as the approximation of uniform internal particle temperature are valid for a particle diameter up to 5-30  $\mu$ m, more than two orders of magnitude greater than the nominal 42 nm particle diameter. Thus particle aggregation is unlikely to invalidate the assumptions underlying the single fluid mixture model described in Chapter 5.

The Schmidt number for the particulate phase governs the importance of viscous diffusion compared to diffusion by Brownian motion. The Schmidt number is calculated from equation A.17 where  $v_g$  is the kinematic viscosity of the fluid phase and  $D_p$  is the Brownian diffusion coefficient for the particles [2].

$$Sc = \frac{V_g}{D_p} \tag{A.17}$$

Figure A.7 provides values of both the particle diffusivity and the corresponding Schmidt number as a function of particle diameter and fluid temperature.



Figure A.7: Particle diffusivity and Schmidt number for  $d_p < 100$  nm

For a particle diameter exceeding 5 nm the Schmidt number reaches values greater than 100 whereas for particle diameter exceeding 15 nm the Schmidt number reaches values greater than 1000 implying that Brownian motion does not likely become relevant until the particle shrinks to less than 40% of its original size.

The relative importance of natural to forced convection in the tubes is given by the Richardson number which, for an ideal gas, is described by equation A.18 with  $T_s$  representing the wall temperature,  $T_{\infty}$  representing fluid temperature distant from the wall and T assumed to be the average temperature [6].

$$Ri = \frac{Gr}{Re^2} = \frac{g(T_s - T_{\infty})D_t}{Tv_{avg}^2}$$
(A.18)

Figure A.8 shows the Richardson number within the tubes as a function of  $T_s$  and the gas flow rate assuming the average velocity corresponds to that from a laminar flow profile at temperature  $T_{\infty}$ . Under these conditions, neither free nor forced convection can be neglected unless  $T_{\infty}$ approaches  $T_s$  or the gas flow rate is high.



Figure A.8: Richardson number in flow tubes

The transition between laminar and turbulent flow in each the tubes and cavity space is dictated by the Reynolds and Grashof numbers respectively. The Reynolds number for flow within the reaction tubes is shown in Figure A.9 as a function of temperature and inert gas flow rate. The flow pattern remains laminar for all reasonable flow rates within the reaction tubes.



Figure A.9: Reynolds number in flow tubes

The transition to turbulent flow for the buoyancy-driven circulating flow in the receiver cavity is related to the Grashof number which, for an ideal gas, is given by equation A.19 where  $T_s$  is taken to be the wall temperature,  $T_{\infty}$  is taken to be the fluid temperature away from the wall and T is assumed to be the average temperature [6].

$$Gr = \frac{\rho^2 g (T_{\infty} - T_s) L^3}{\mu^2 T}$$
(A.19)

Figure A.10 shows the Grashof number as a function of the heated fluid temperature near the tubes with a constant wall surface temperature of 300 K when the characteristic length is taken to be the cavity radius. For purely buoyancy driven flow the transition to turbulence is typically described as taking place at  $Gr \approx 10^8 - 10^9$ , well above the values shown in Figure A.10.



Figure A.10: Grashof number in cavity fluid

#### References

- 1. Weimer, A.W. and Clough, D.E., Modeling of Char Particle Size-Conversion Distributions in a Fluidized-Bed Gasifier Non-Isothermal Effects. *Powder Technology*, 1980. **27**(1): p. 85-103.
- 2. Hinds, W.C., *Aerosol Technology*. 1982, New York: John Wiley and Sons.
- 3. Rosner, D.E. and Park, H.M., Thermophoretically Augmented Mass-Transfer Momentum-Transfer and Energy-Transfer Rates in High Particle Mass Loaded Laminar Forced-Convection Systems. *Chemical Engineering Science*, 1988. **43**(10): p. 2689-2704.
- 4. Ishii, M. and Hibiki, T., *Thermo-Fluid Dynamics of Two-Phase Flow*. 2006, New York: Springer Science-Business Media.
- 5. Ishii, M. and Mishima, K., 2-Fluid Model and Hydrodynamic Constitutive Relations. *Nuclear Engineering and Design*, 1984. **82**(2-3): p. 107-126.
- 6. Bird, R.B., Stewart, W.E., and N., L.E., *Transport Phenomena*. 2 ed. 2002, New York: John Wiley and Sons, Inc.
- 7. Maag, G., Lipinski, W., and Steinfeld, A., Particle-gas reacting flow under concentrated solar irradiation. *International Journal of Heat and Mass Transfer*, 2009. **52**(21-22): p. 4997-5004.
- 8. Lipinski, W., Thommen, D., and Steinfeld, A., Unsteady radiative heat transfer within a suspension of ZnO particles undergoing thermal dissociation. *Chemical Engineering Science*, 2006. **61**(21): p. 7029-7035.
- 9. Laurendeau, N.M., Heterogeneous Kinetics of Coal Char Gasification and Combustion. *Progress in Energy and Combustion Science*, 1978. **4**(4): p. 221-270.

## **Appendix B**:

# Comparison of fluid properties predicted by correlations with literature data

#### **B.1** Chapman Enskog, Eucken, and modified Eucken models

The Chapman-Enskog models are given by equation B.1-B.3 for gas-phase viscosity, thermal conductivity and binary diffusivity [1].

$$\mu (kg/m/s) = 2.6693 \times 10^{-6} \frac{\sqrt{MT}}{\sigma_c^2 \Omega_{\mu}}$$
(B.1)

$$k(W/m/K) = 0.0833 \frac{\sqrt{T/M}}{\sigma_c^2 \Omega_k}$$
(B.2)

$$D_{AB}(m^2/s) = 1.8583 \times 10^{-7} \sqrt{T^3 \left(\frac{1}{M_A} + \frac{1}{M_B}\right)} \frac{1}{p \sigma_{AB}^2 \Omega_D}$$
(B.3)

In equations B.1-B.3  $\sigma_c$  is the collision diameter (Å),  $\Omega$  is the collision integral, *T* is the local temperature (K), *p* is the local pressure (atm) and *M* is the molecular weight. The collision diameter in equation B.3 is approximated as the average of the collision diameters of molecules A and B [1]. Chapman-Enskog theory produces stronger temperature dependence than kinetic theory and, though equations B.1-B.3 are only strictly valid for non-polar monatomic gases at low density, viscosity and diffusivity equations tend to produce acceptable results for a variety of non-polar and polyatomic gases.

The Eucken and modified Eucken correlations are semi-empirical equations that account for changes in internal rotational and vibrational energy due to molecular collisions, and thereby produce more accurate thermal conductivity predictions for polyatomic gases. The Eucken and

$$k = \left(\frac{C_p}{M} + \frac{5}{4}\frac{R}{M}\right)\mu \tag{B.4}$$

$$k = \left(1.32\frac{C_p}{M} + 0.88\frac{R}{M}\right)\mu\tag{B.5}$$

#### **B.2** Comparison of model predictions with literature data

Figures B.1 and B.2 present the Chapman-Enskog calculations for CO, H<sub>2</sub>, CO<sub>2</sub>, and Ar viscosity alongside available literature data [2-4]. The Chapman-Enskog models agree well with literature data for CO, H<sub>2</sub>, CO<sub>2</sub>, and Ar with predicted viscosity differing by at most 5% from literature data for T < 800 K (CO and CO<sub>2</sub>) or T < 1600 K (Ar and H<sub>2</sub>).





Figure B.3 provides Chapman-Enskog calculations for binary diffusivity of dilute CO or  $H_2$  in argon at atmospheric pressure. The Chapman-Enskog models again agree well with literature data [2] for temperatures below 700 K with predicted diffusivities differing from literature data by at most 5% for CO and 10% for  $H_2$ .



Figure B.3: Binary diffusivity of dilute carbon monoxide or hydrogen in argon

Figures B.4-B.7 present Chapman-Enskog, Eucken, and modified Eucken calculations for CO, H<sub>2</sub>, CO<sub>2</sub>, and Ar thermal conductivity along with literature data for temperatures up to

800-1600 K [2, 3, 5]. Eucken and modified Eucken model calculations are carried out with viscosity predicted by Chapman-Enskog theory. Chapman-Enskog models clearly fail to accurately capture the temperature dependence of thermal conductivity for polyatomic components and only yield reasonable solutions for argon where thermal conductivity predictions accurate to within 6% of literature values are obtained. Chapman-Enskog predictions of CO thermal conductivity for temperatures up to 800 K yield errors on the order of 30-40% whereas modified Eucken predictions are accurate to within 4%.



Figure B.4: Carbon monoxide thermal conductivity

The modified Eucken correlation also generates superior predictions of the thermal conductivity for  $H_2$  and  $CO_2$  with less than 10% discrepancy between theoretically predicted values and literature data. Chapman-Enskog correlations over an identical temperature range yield errors as high as 140%. Predictions from modified Eucken models are superior to those from Eucken models for each of the polyatomic molecules at high temperature. However, Chapman-Enskog models are adequate for monatomic species such as argon.



Figure B.5: Hydrogen thermal conductivity



Figure B.6: Carbon dioxide thermal conductivity



Figure B.7: Argon thermal conductivity

### References

- 1. Bird, R.B., Stewart, W.E., and N., L.E., *Transport Phenomena*. 2 ed. 2002, New York: John Wiley and Sons, Inc.
- 2. Haynes, W.M., ed. *CRC Handbook of Chemistry and Physics*. 91st ed. 2010, CRC Press / Taylor and Francis: Boca Raton, FL.
- 3. Incropera, F.P. and Dewitt, D.P., *Fundamentals of Heat and Mass Transfer*. 5th ed. 2002, New York: John Wiley and Sons.
- 4. Dawe, R.A. and Smith, E.B., Viscosity of Argon at High Temperatures. *Science*, 1969. **163**(3868): p. 675-&.
- 5. Poling, B.E., Prausnitz, J.M., and O'Connel, J.P., *The Properties of Gases and Liquids*. 5th ed. 2001, New York: McGraw-Hill.

# Appendix C:

## Specification of tube positions for optimization

#### C.1 Method A

All designs are created relative to a base design with the tubes arranged in a semicircle around the back cavity wall. Geometric factors allow for variations in the number of tubes as well as the size and position of the tubes and are illustrated in Figure 6.1. Geometric parameters are specified as in Figure 6.2. For this study tube size is determined from a specified maximum tube surface area per unit length ( $A_{max}$ ) with  $A_{max}$  proportional to the cavity size. For this study the ratio  $A_{max}/r_{cav} = 5.6$  is chosen arbitrarily in order to generate physically realistic designs. The variable  $r_{t,max}$  refers to the maximum radius of each outer tube and is calculated in equation C.1 for the "outer" semicircle with tubes in the "inner" semicircle having identical size.

$$r_{t,\max} = \frac{f_2 A_{\max}}{2\pi [(N_{\max} - 1) + f_r^{1/2}]} \qquad A/A_{max} = 1 \tag{C.1}$$

As tube removal must be performed in an integer number, the maximal tube radius is allowed to vary slightly between designs having  $A/A_{max} = 1$  and  $A/A_{max} < 1$  in equation C.2 where N is the number of tubes after removal from the ends of the array and is determined such that  $N/N_{max}$  is as close as possible to  $A/A_{max}$ .

,

$$r_{t,\max} = \frac{f_2 A_{\max} \left(\frac{A}{A_{\max}}\right)}{2\pi \left[ (N-1) + f_r^{1/2} \right]} \qquad A/A_{\max} < 1 \tag{C.2}$$

Factor levels are chosen such that the array always contains an odd number of tubes. Thus a space between tubes never occurs directly at the back of the cavity and excessive heat load on

the back cavity wall from direct solar incidence is avoided. For this reason  $N_{max}$  is restricted to either 5 or 9. For  $A/A_{max} = 0.6$ , the modified tube arrays have 3 and 5 tubes, respectively, and the difference between the two calculations of  $r_{t,max}$  from equations C.1 and C.2 is at most 8%.

The maximum radius of the outer tube circle is calculated from equations C.3 and C.4 assuming the maximal tube radius is given by the calculation in equation C.1.

$$r_{o,\max} = r_{cav} - d_w - \frac{A_{\max} f_r^{1/2}}{2\pi (N_{\max} - 1 + f_r^{1/2})}$$
(C.3)

$$r_o = f_2 r_{o,\max} \tag{C.4}$$

The "inner" tube circle radius is determined geometrically from Figure 6.2(b) and written in equation C.5.

$$r_{i} = r_{o} \left[ 1 + \frac{f_{1}^{2}}{2(1 - f_{1})} \right]$$
(C.5)

Therefore the actual tube circle radius utilized in the design is given by equation C.6.

$$r_{c} = f_{2}r_{o,\max}\left[1 + \frac{f_{1}^{2}}{2(1 - f_{1})}\right]$$
(C.6)

Each tube is assigned an index *i* in a counter-clockwise fashion with the tube at the rightmost end of the array denoted by i = 1. For designs with staggered tube patterns the even-numbered tubes remain on the circle with radius  $r_c$  whereas the odd-numbered tubes are moved inward onto a circle with radius  $r_{c.s}$  given by equation C.7.

$$r_{c,s} = r_c (1 - f_s)$$
 (C.7)

Assuming uniform spacing between tubes in the array, the distance along the arc between tube walls can be calculated from equation C.8.

$$d_{t} = \frac{2r_{c}\sin^{-1}\left[\frac{2(1-f_{1})}{(f_{1}-1)^{2}+1}\right] - 2r_{c}\left[\left(N_{\max}-2\right)\tan^{-1}\left(\frac{r_{t,\max}}{r_{c}}\right) + \tan^{-1}\left(\frac{r_{t,\max}}{r_{c}}\right)\right]}{N_{\max}-1}$$
(C.8)

The angular coordinate of a given tube center is defined relative to the tube circle with angle  $\theta$  measured from the positive *x*-axis. Angular tube coordinates are calculated based on the tube index using equations C.9-C.11.

$$\theta_{i} = \frac{\pi}{2} - \sin^{-1} \left[ \frac{2(1 - f_{1})}{(f_{1} - 1)^{2} + 1} \right] + \left( \frac{N_{\max} - N}{2} + i - 1 \right) \left[ \frac{d_{t}}{r_{c}} + 2 \tan^{-1} \left( \frac{r_{t,\max}}{r_{c}} \right) \right] \quad i < \frac{N + 1}{2} \tag{C.9}$$

$$\theta_i = \frac{\pi}{2} \qquad \qquad i = \frac{N+1}{2} \qquad (C.10)$$

$$\theta_{i} = \frac{\pi}{2} + \sin^{-1} \left[ \frac{2(1-f_{1})}{(f_{1}-1)^{2}+1} \right] - \left( \frac{N_{\max}+N}{2} - i \right) \left[ \frac{d_{t}}{r_{c}} + 2\tan^{-1} \left( \frac{r_{t,\max}}{r_{c}} \right) \right] \qquad i > \frac{N+1}{2} \qquad (C.11)$$

The (x,y) positions of each tube center are determined in relation to the coordinate system in Figure 6.2(c) with (0,0) defined as the cavity center point. The tube circle is centered at  $(x_{c,o}, y_{c,o})$  where  $x_{c,o} = 0$  and  $y_{c,o}$  is given by equation C.12.

$$y_{c,o} = -\frac{f_1 f_2 r_{o,\max}}{2} \frac{(2 - f_1)}{(1 - f_1)}$$
(C.12)

Finally (x, y) coordinates for the center of tube *i* are given by equations C.13 and C.14.

$$x_i = r_{c,i} \cos(\theta_i) + x_{c,o} \tag{C.13}$$

$$y_i = r_{c,i} \sin(\theta_i) + y_{c,o} - f_o r_{cav}$$
 (C.14)

The tube circle radius used in equations C.13 and C.14 is determined based on the even/odd staggering of the tube array in equations C.15 and C.16.

$$r_{c,i} = r_c \quad \text{even } i \tag{C.15}$$

$$r_{c,i} = r_{c,s} \quad \text{odd } i \tag{C.16}$$

The tube radius used in the simulations is a fraction of the maximal tube radius determined from equation C.1 or C.2. The radius of the center tube (equation C.18) may be larger than that of the outer tubes (equation C.17) for  $f_r > 1$ .

$$r_{t,i} = r_{t,\max}\left(\frac{r}{r_{\max}}\right) \qquad \qquad i \neq \frac{N+1}{2} \qquad (C.17)$$

$$r_{t,i} = r_{t,\max} f_r^{1/2} \left( \frac{r}{r_{\max}} \right)$$
  $i = \frac{N+1}{2}$  (C.18)

#### C.2 Method B

The second method of specifying tube positions eliminates parameters  $f_1$  and  $A/A_{max}$  while adding an additional parameter  $\theta_c$  shown in Figure 6.3. The number of tubes in the array is now  $N_{max}$ . Parameters  $f_s$  and  $f_o$  are defined as shown in Figures 6.2(c) and 6.2(d). Unlike in Method A, the distance  $d_t$  between individual tubes along the tube circle is fixed and the maximum tube radius is determined from this distance and angle  $\theta_c$ . The maximal radius of the tube circle is given as in Method A from equation C.19 and the actual radius of the tube circle is calculated from equation C.20.

$$r_{o,\max} = r_{cav} - d_w - r_{t,\max} \tag{C.19}$$

$$r_c = f_2 r_{o,\max} \tag{C.20}$$

The maximum tube radius  $(r_{t,max})$  is then determined by solving the implicit equation C.21.

$$\theta_c = 2(N-1)\tan^{-1}\left(\frac{r_{t,\max}}{r_c}\right) + 2\tan^{-1}\left(\frac{r_{t,\max}f_r^{1/2}}{r_c}\right) + (N-1)\frac{d_t}{r_c}$$
(C.21)

Angular coordinates corresponding to the positions of the tube centers are again defined relative to the center of the tube semicircle and measured from the positive *x*-axis. These coordinates are specified in equations C.22 - C.24.

$$\theta_{i} = \frac{\pi - \theta_{c}}{2} + 2\left(i - \frac{1}{2}\right) \tan^{-1}\left(\frac{r_{t,\max}}{r_{c}}\right) + (i - 1)\frac{d_{t}}{r_{c}} \qquad i < \frac{N+1}{2} \qquad (C.22)$$

$$\theta_i = \frac{\pi}{2} \qquad \qquad i = \frac{N+1}{2} \qquad (C.23)$$

$$\theta_{i} = \frac{\pi + \theta_{c}}{2} - 2\left(N - i + \frac{1}{2}\right) \tan^{-1}\left(\frac{r_{t,\max}}{r_{c}}\right) - \left(N - i\right)\frac{d_{t}}{r_{c}} \qquad i > \frac{N+1}{2} \qquad (C.24)$$

The (x,y) positions of each tube center are again determined in relation to the coordinate system in Figure 6.2(c) with (0,0) defined as the cavity center point. The tube circle is centered at  $(x_{c,o}, y_{c,o}) = (0,0)$  and the tube (x,y) coordinates are given by equations C.13 – C.16 with tube radius given by equations C.17 and C.18.

## **Appendix D**

# Tube configurations, operating conditions, and results for optimization studies

#### **D.1 Reflective cavity**

Tables D.1 – D.6 list operating conditions, cavity size, and number of tubes for receiver designs examined as part of the optimization studies in Chapter 6. Tube configurations are specified with eight individual factors and schematic depictions for the tube configurations for each design are given in Figures D.1 - D.5. All receiver configurations are generated using the factor levels discussed in Chapter 6. Table D.1 and Figure D.1 represent at resolution IV 2<sup>13-8</sup> fractional factorial design with tube positions specified using method A in Appendix C with factor  $f_r$  held constant at  $f_r = 1$ . Table D.2 and Figure D.2 represent a resolution IV  $2^{6-2}$  fractional factorial design. Tube positions are again specified via method A with  $f_r = 1$ ,  $f_o = 0$ ,  $r_{cav} = 3.6$  in, and  $h_{cav} = 8$  in. Operating conditions are held constant at  $R_I = 1$  s<sup>-1</sup>,  $C_{feed} = 6$  g/min,  $R_{steam} = 1$ , and  $Q_s = 7$  kW. Tables D.3 and D.4 and Figure D.3 are a resolution IV  $2^{8-4}$  fractional factorial design with tube positions specified using method A and  $f_o = 0$ ,  $f_s = 0$ ,  $f_l = 0$ , and  $h_{cav} = 8$  in. Operating conditions constant for all simulations are  $R_I = 1$  s<sup>-1</sup> and  $R_{steam} = 1$ . Tables D.3 and D.4 contain results for solar power inputs ranging between 6-7 kW and 7-8 kW respectively. Table D.5 and Figure D.4 are a resolution IV 2<sup>4-1</sup> fractional factorial design with tube positions specified using method B in Appendix C with  $f_o = 0$ ,  $f_s = 0$ ,  $\theta_c = 90^\circ$ ,  $h_{cav} = 8$  in, and  $r_{cav} = 3.6$  in. Operating conditions are held constant at  $R_I = 0.75 \text{ s}^{-1}$ ,  $C_{feed} = 6 \text{ g/min}$ ,  $R_{steam} = 1$ , and  $Q_s = 7 \text{ kW}$ . Tables D.6 and Figure D.5 are a five factor face-centered central composite design based on a resolution V half fraction of a five-factor factorial. Tube positions are specified via method B

with  $f_o = 0$ ,  $f_s = 0$ ,  $\theta_c = 90^\circ$ ,  $h_{cav} = 8$  in,  $r/r_{max} = 1$ ,  $f_I = 0$ , N = 3 and constant operating conditions are  $R_I = 0.5$  s<sup>-1</sup>, and  $R_{steam} = 1$ .

#### **D.2** Absorbing cavity

Tables D.7 – D.11 list operating conditions, cavity size, and number of tubes for receiver designs investigated as part of the optimization studies in Chapter 7. Tube configurations are specified with eight individual factors and schematic depictions for the tube configurations for each design are given in Figures D.6 - D.9. All receiver configurations are generated using the factor levels discussed in Chapter 7. Table D.7 represents a resolution IV  $2^{13.8}$  fractional factorial design identical to that in Table D.1. Tube positions are identical to those in Figure D.1. Table D.8 and Figure D.6 represent a resolution IV  $2^{6-2}$  fractional factorial design. Tube positions are again specified via method A with  $f_o = 0$ ,  $f_I = 0$ ,  $r_{cav} = 3.6$  in, and  $h_{cav} = 8$  in. Operating conditions are held constant at  $R_I = 0.5$  s<sup>-1</sup>,  $C_{feed} = 6$  g/min,  $R_{steam} = 1$ , and  $Q_s = 7$  kW. Table D.9 and Figure D.7 represent a five factor face-centered central composite design based on a resolution V half fraction of a five-factor factorial. Tube positions are specified by method B with  $f_o = 0$ ,  $f_I = 0$ ,  $r/r_{max} = 1$ ,  $f_2 = 1$ ,  $f_r = 1$  and  $h_{cav} = 8$  in. Operating conditions held constant are  $R_I = 0.25$  s<sup>-1</sup>, and  $R_{steam} = 1.25$ .

																										r							
	$\max_{(kW/m^2)} q_{abs,s}$	1278	1157	723	1137	560	1123	803	766	1109	386	566	741	853	783	1199	394	1829	280	436	539	658	707	1117	494	728	444	326	822	369	1055	LLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLL	732
	$egin{array}{c} T_{min} \ ({ m K}) \end{array}$	1557	1296	1091	1445	1342	1713	1377	1052	1712	1203	1294	1249	1588	1430	1573	812	1485	1145	1144	1078	1265	1321	1417	939	1383	1302	832	1287	1164	1589	1367	967
	$T_{max}$ (K)	1858	1753	1544	1927	1456	1855	1683	1665	1872	1460	1604	1678	1752	1577	1910	1427	1988	1410	1596	1537	1625	1686	1894	1457	1663	1531	1324	1767	1398	1877	1708	1652
	$\stackrel{X_{avg}}{(00)}$	23	4	2	17	1	17	8	9	26	Э	1	7	11	1	19	0.3	20	1	S	1	9	9	12	1	7	С	0.01	16	0.4	21	4	
cavity	$X_{max}$ (%)	45	17	10	44	7	23	18	30	4	12	9	20	21	7	38	7	51	4	22	5	17	18	43	7	7	11	0.04	51	1	34	13	7
flective	$\eta_2$ (%)	23.8	31.7	43.3	27.7	28.0	14.3	24.7	27.0	28.0	29.9	37.8	32.0	23.8	38.1	44.4	48.9	32.0	31.1	38.8	38.5	40.0	36.4	43.0	50.8	49.4	52.1	69.8	51.1	50.2	30.6	42.3	52.4
(2 <sup>13-8</sup> ): re	(%) 1/4	12.2	3.0	1.5	5.4	1.1	10.3	3.8	5.8	22.9	1.3	0.3	7.4	2.4	0.5	10.3	0.1	15.9	0.4	1.0	1.1	1.1	6.3	7.1	0.2	0.6	1.4	0.003	2.6	0.2	5.7	1.0	0.5
Design 1 (	$\eta_{abs, net}$ (%)	29.6	37.3	50.6	34.3	36.2	20.2	34.1	37.7	34.5	41.0	48.8	41.7	43.4	42.5	49.4	56.8	39.1	44.1	50.5	49.6	46.1	42.8	49.5	60.2	56.4	60.7	77.8	58.2	61.4	38.0	53.5	65.1
esults for	$\eta/\eta_{max, C}$ (%)	23.9	4.3	2.2	17.9	0.9	17.1	8.0	6.8	25.9	3.6	1.4	6.9	11.5	0.6	19.4	0.3	21.3	1.1	5.1	1.3	6.4	6.8	13.1	1.1	2.6	3.2	0.003	17.0	0.4	21.2	3.8	1.2
e D.1: R	(%) 1/2	2.9	0.9	0.7	1.5	0.3	1.5	0.9	1.6	6.4	0.4	0.1	2.4	0.9	0.2	4.6	0.03	5.1	0.1	0.4	0.4	0.5	2.3	3.0	0.1	0.3	0.7	0.002	1.3	0.1	1.7	0.4	0.2
Tabl	$r_{cav}$ (cm)	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2
	$r_t$ (cm)	0.58	0.58	0.97	0.32	0.97	0.35	0.58	0.54	0.97	0.97	1.62	0.54	1.62	0.58	0.97	06.0	0.97	0.97	1.62	0.54	1.62	0.58	0.97	06.0	1.62	1.62	2.70	0.90	2.70	0.97	1.62	1.50
	$C_{feed}$ (g/min)	2	9	9	7	9	7	2	9	9	2	7	9	7	9	9	2	9	7	7	9	7	9	9	7	2	9	9	7	9	7	7	9
	$(k_{W})$	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0
	N	Э	5	5	6	e	5	5	6	Э	5	5	6	ŝ	S	5	6	3	5	S	6	e	5	S	6	ŝ	S	5	6	e	5	S	6
	Design	1	2	ε	4	5	9	7	8	6	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32
-																		-														_	



Figure D.1: Tube configurations for Design 1  $(2^{13-8})$ : reflective or absorbing cavity

	Max $q^{"}_{abs,s}$ (kW/m <sup>2</sup> )	1887	1434	970	872	913	796	1176	1004	1387	1118	1169	1079	1149	1042	986	1081
	$T_{min}(\mathbf{K})$	1695	1565	1617	1291	1588	1300	1651	1391	1615	1429	1784	1599	1685	1462	1585	1280
	$T_{max}\left(\mathbf{K}\right)$	2034	1920	1841	1790	1882	1751	1929	1850	1924	1895	1896	1880	1827	1925	1824	1860
cavity	$X_{avg}$ (%)	21.8	18.0	23.2	10.2	21.3	11.6	23.9	16.9	26.3	17.6	29.0	24.0	7.6	9.8	24.7	14.8
reflective (	$X_{max}$ (%)	41.8	44.2	39.7	31.9	42.0	31.0	46.1	40.2	52.2	53.3	36.5	39.4	11.3	25.3	36.5	44.5
gn 2 (2 <sup>6-2</sup> ):	$\eta_2$ (%)	26.3	32.4	46.5	55.9	32.9	39.7	32.6	39.4	34.7	42.5	34.0	42.4	22.1	29.9	42.9	52.1
ts for Desig	(%) 1 <sup>1</sup>	21.3	14.0	12.0	4.4	16.3	7.1	18.4	10.6	19.0	10.1	21.2	13.8	8.6	8.3	14.0	6.9
D.2: Resul	$\eta_{abs,  net} \ (\%)$	30.9	38.4	52.5	62.9	39.2	46.8	37.1	45.3	40.0	49.0	38.2	47.6	26.3	35.5	48.0	59.1
Table	η/η <sub>max, C</sub> (%)	22.4	18.5	23.5	10.7	21.7	12.1	24.2	17.3	27.0	18.4	29.1	24.3	7.7	10.1	24.9	15.6
	(%) 1	3.4	2.8	3.6	1.6	3.3	1.8	3.7	2.7	4.1	2.7	4.6	3.7	1.2	1.5	3.9	2.3
	$r_t$ (cm)	0.58	0.58	1.62	1.62	0.58	0.54	0.58	0.54	0.97	0.97	0.97	0.97	0.35	0.32	0.97	0.90
	N	ю	S	e	5	S	6	S	6	Э	S	ξ	S	S	6	5	6
	Design	1	7	б	4	5	9	٢	8	6	10	11	12	13	14	15	16



Table D.3: Results for Design 3  $(2^{8-4})$ : reflective cavity with 6-7 kW solar power

$\max_{(kW/m^2)} q_{abs,s}$	1589	1124	585	735	474	962	1176	555	1002	537	664	1042	1287	1181	721	567
$\begin{array}{c} T_{min} \\ ({ m K}) \end{array}$	1660	1285	1411	1205	1325	1329	1651	1104	1568	1095	1511	1685	1508	1435	1497	1078
$\begin{array}{c}T_{max}\ ({ m K})\end{array}$	1979	1873	1648	1701	1527	1772	1929	1641	1854	1607	1656	1896	1952	1858	1726	1609
$X_{avg}$ (%)	34.6	13.3	4.9	5.7	6.7	21.9	23.9	7.1	34.1	7.7	11.5	33.9	38.4	5.6	23.2	3.3
X <sub>max</sub> (%)	58.5	49.6	11.7	20.6	10.2	52.6	46.1	35.0	44.7	16.4	14.0	41.0	57.4	7.7	28.6	7.4
$\eta_2^{(\%)}$	22.6	34.7	49.6	57.4	37.4	37.4	32.6	42.0	36.3	47.3	38.4	39.1	23.5	31.0	42.0	58.7
η <sub>1</sub> (%)	15.8	9.6	0.7	2.8	5.0	4.8	18.4	1.6	23.2	1.5	8.2	7.1	14.2	8.6	5.3	2.0
$\eta_{abs, net}$ (%)	27.7	41.0	57.0	64.8	44.5	44.7	37.1	49.7	41.7	55.0	44.7	44.8	29.3	37.6	48.7	67.0
η/η <sub>max, C</sub> (%)	35.4	14.4	5.0	6.0	6.8	22.8	24.2	7.7	34.5	8.2	11.5	33.9	39.4	6.3	23.2	4.1
(%) 4	2.2	2.1	0.3	1.1	1.3	1.1	3.7	0.4	5.2	0.5	2.1	1.7	2.0	1.7	1.4	0.8
$r_{cav}$ (cm)	9.1	12.2	12.2	9.1	12.2	9.1	9.1	12.2	9.1	12.2	12.2	9.1	12.2	9.1	9.1	12.2
$f_r$	-	-	1	-	-	-	1	-	З	ŝ	ω	ŝ	ω	ŝ	ε	ŝ
Outer $r_i$ (cm)	0.58	0.78	2.16	1.62	0.78	0.54	0.58	0.72	0.78	1.13	1.04	0.85	0.41	0.30	0.85	1.11
C <sub>feed</sub> (g/min)	2	9	0	9	9	0	9	0	9	0	9	0	0	9	0	9
$\overset{(kW)}{O_s}$	9	7	7	9	9	7	7	9	7	9	9	7	7	9	9	7
Ν	з	5	ε	5	5	6	5	6	З	5	e	5	5	6	5	6
Design	1	7	б	4	5	9	7	8	6	10	11	12	13	14	15	16

	$\max_{(kW/m^2)} q_{abs,s}$	2185	1124	585	1011	653	796	1176	764	1002	739	913	1042	1287	1625	992	567	/0c
	$T_{min}$ (K)	1821	1285	1411	1363	1467	1329	1651	1252	1568	1236	1667	1685	1508	1607	1649	1078	
	$T_{max}$ (K)	2170	1873	1648	1869	1676	1772	1929	1802	1854	1760	1813	1896	1952	2040	1892	1609	
	$X_{avg}$ (%)	53.1	13.3	4.9	15.8	18.5	21.9	23.9	17.4	34.1	18.8	28.0	33.9	38.4	13.9	46.5	3.3	
	$X_{max}$ (%)	74.7	49.6	11.7	42.4	25.6	52.6	46.1	57.3	44.7	38.1	32.2	41.0	57.4	20.7	52.6	7.4	14
	$\eta_2$ (%)	20.5	34.7	49.6	54.7	34.6	37.4	32.6	39.2	36.3	44.4	36.7	39.1	23.5	28.7	39.5	58.7	): reflect
	(%) 1μ	20.0	9.6	0.7	6.0	11.1	4.8	18.4	3.1	23.2	3.0	15.9	7.1	14.2	16.2	8.5	2.0	$\begin{array}{c} 2.0 \\ 1.0 \\ 1.0 \\ 2.5 \\$
	$\eta_{abs, net}$ $(\%)$	25.1	41.0	57.0	61.3	40.9	44.7	37.1	46.2	41.7	51.3	41.7	44.8	29.3	34.4	45.0	67.0	or Desig
~	$\eta/\eta_{max,C}$ (%)	53.8	14.4	5.0	16.4	18.7	22.8	24.2	18.3	34.5	19.8	28.0	33.9	39.4	14.4	46.6	4.1	$\begin{array}{c} 4.1 \\ 0 \\ 12 \\ 12 \\ 12 \\ 12 \\ 12 \\ 12 \\ 12$
	(%) μ	2.4	2.1	0.3	2.1	2.5	1.1	3.7	0.8	5.2	0.8	3.8	1.7	2.0	2.8	2.1	0.8	U.S Config
	$r_{cav}$ (cm)	9.1	12.2	12.2	9.1	12.2	9.1	9.1	12.2	9.1	12.2	12.2	9.1	12.2	9.1	9.1	12.2	3: Tube
	$f_r$	1	1	1	-	1	1	1	1	Э	Э	ε	ε	ε	ε	Э	Э	c d d d d d d d d d d d d d d d d d d d
	Outer $r_t$ (cm)	0.58	0.78	2.16	1.62	0.78	0.54	0.58	0.72	0.78	1.13	1.04	0.85	0.41	0.30	0.85	1.11	
	$C_{feed}$ (g/min)	2	9	7	9	9	2	9	2	9	2	9	7	7	9	7	9	
	$Q_{\rm s}$ (kW)	7	8	8	7	7	8	8	7	8	7	7	8	8	7	7	8	
	N	з	5	З	5	5	6	5	6	З	5	ω	5	5	6	5	6	
	Design	1	7	З	4	5	9	7	8	6	10	11	12	13	14	15	16	<u>e</u>

Table D.4: Results for Design 3  $(2^{8-4})$ : reflective cavity with 7-8 kW solar power

$\max q^{"}_{abs,s}$ (kW/m <sup>2</sup> )	2028	861	006	1526	856	1635	2229	866
$T_{min}$ (K)	1741	1715	1692	1738	1614	1659	1685	1635
$T_{max}(\mathbf{K})$	2058	1798	1842	1924	1788	2046	2097	1788
$X_{avg}$ (%)	23.6	32.3	34.4	34.2	22.5	19.9	13.8	30.3
$X_{max}$ (%)	42.8	36.1	39.5	41.1	31.2	44.1	18.1	34.3
$\eta_2$ (%)	26.1	43.2	35.1	31.1	33.5	28.3	23.4	40.4
(%) 1μ	23.4	18.2	24.1	27.7	16.7	18.0	15.0	18.4
$\eta_{abs, net}$	30.2	48.3	40.4	35.1	39.2	32.5	24.3	45.7
η/η <sub>max, C</sub> (%)	24.2	32.3	34.4	34.3	22.7	20.4	13.8	30.4
(%) 4	3.7	5.1	5.3	5.3	3.5	3.1	2.2	4.7
Outer $r_t$ (cm)	0.56	1.43	0.78	0.63	0.61	0.46	0.27	0.74
$f_r$	1	1	2.5	2.5	1	1	2.5	2.5
Ν	з	б	б	б	5	5	5	5
Design	1	7	С	4	5	9	٢	8







Table D.6: Results for Design 5 (face-centered central composite): reflective cavity

																								_			
$\max_{(kW/m^2)} q_{abs,s}$	1989	1116	2099	1271	1074	827	1084	828	2295	1288	2422	1466	1239	954	1250	956	1383	1001	1211	1378	1806	943	1213	1400	1307	1307	1307
$egin{array}{c} T_{min} \ ({ m K}) \end{array}$	1782	1829	1830	1786	1708	1656	1663	1672	1912	1867	1866	1901	1747	1748	1769	1718	1782	1767	1781	1768	1851	1711	1738	1813	1795	1760	1776
$T_{max}$ (K)	2064	1982	2107	1917	1860	1753	1807	1793	2209	2018	2139	2046	1896	1848	1929	1843	1994	1896	1929	1917	2028	1839	1881	1960	1945	1901	1921
$\substack{X_{avg} \\ (\%)}$	20	52	43	32	41	25	25	39	48	41	28	62	32	49	53	34	39	43	42	42	44	38	38	47	50	34	42
$X_{max}$ (%)	30	62	48	35	55	27	30	41	61	50	32	99	45	52	60	35	48	46	51	47	52	42	44	53	22	39	49
$\eta_2^{(\%)}$	30.0	33.6	25.0	37.7	32.2	44.3	35.8	39.9	24.5	37.4	28.6	31.9	35.4	39.9	30.8	42.3	31.4	39.0	35.9	35.4	32.4	38.1	36.1	35.0	33.1	37.5	35.5
$\eta_{l}$	25.0	28.7	32.2	30.8	23.0	19.4	24.7	17.2	33.1	35.1	31.5	31.9	28.3	19.0	27.4	24.5	31.7	27.5	29.2	30.3	35.2	24.4	28.0	31.7	25.8	29.8	30.0
η <sub>abs, net</sub> (%)	33.6	38.1	28.7	41.9	37.0	49.6	40.3	39.9	28.1	41.3	31.9	35.9	39.6	45.0	35.1	47.3	31.4	43.7	40.3	39.7	36.3	43.1	40.6	39.3	37.6	41.8	39.9
$\eta/\eta_{max,C}^{(\%)}$	20.8	52.5	42.7	32.4	41.7	25.0	25.4	39.5	48.6	41.4	28.2	62.2	32.6	49.0	53.5	34.3	39.2	43.0	41.8	42.5	44.5	37.6	37.7	47.0	50.3	33.8	42.4
μ (%)	5.7	9.7	8.0	11.6	7.4	8.6	8.9	6.9	8.1	13.1	9.0	10.2	10.0	7.6	8.5	10.3	10.0	10.7	10.5	10.7	11.4	9.3	10.1	11.1	8.5	11.2	10.7
$r_{cav}$ (cm)	6.60	6.60	6.60	6.60	9.14	9.14	9.14	9.14	6.60	6.60	6.60	6.60	9.14	9.14	9.14	9.14	7.87	7.87	7.87	7.87	6.60	9.14	7.87	7.87	7.87	7.87	7.87
$r_t$ (cm)	0.50	0.78	0.41	0.64	0.84	1.26	0.68	1.04	0.50	0.78	0.41	0.64	0.84	1.26	0.68	1.04	09.0	0.91	0.85	0.69	0.57	0.94	0.76	0.76	0.76	0.76	0 76
$f_r$	1.5	1.5	б	ς	1.5	1.5	ю	б	1.5	1.5	б	б	1.5	1.5	б	б	2.25	2.25	1.5	ε	2.25	2.25	2.25	2.25	2.25	2.25	2.25
$C_{feed}$ (g/min)	8	4	4	8	4	8	8	4	4	8	8	4	8	4	4	8	9	9	9	9	9	9	9	9	4	8	9
$Q_s^{o}$	6.5	6.5	6.5	6.5	6.5	6.5	6.5	6.5	7.5	7.5	7.5	7.5	7.5	7.5	7.5	7.5	7	7	7	7	7	7	6.5	7.5	L	7	7
Geom.	1	7	б	4	5	9	7	8	-	2	б	4	5	9	7	8	6	10	11	12	13	14	15	15	15	15	15
Design	1	7	ε	4	5	9	L	8	6	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27





	$\max_{(kW/m^2)} q_{abs,s}$	653	539	366	1105	524	1129	783	543	963	353	541	734	824	772	1217	383	1000	270	422	515	501	700	1118	475	717	423	313	800	359	1028	771	716
	$T_{min}$ (K)	1815	1769	1518	1939	1586	2024	1669	1668	1955	1580	1723	1559	1937	1697	1843	1515	1806	1551	1718	1471	1813	1655	1807	1522	1696	1725	1203	1816	1443	1935	1622	1477
	$T_{max}$ (K)	1863	1850	1618	2106	1671	2076	1843	1846	2020	1669	1846	1801	2017	1809	2066	1706	1984	1639	1873	1712	1920	1802	2067	1710	1846	1826	1468	2112	1566	2108	1852	1809
	$\stackrel{X_{avg}}{(0^{\prime 0})}$	59	42	26	68	26	72	53	61	69	59	56	37	78	21	75	26	72	35	73	20	78	35	67	51	45	68	-	92	19	79	43	33
cavity	X <sub>max</sub> (%)	60	44	31	71	28	74	58	64	70	62	62	44	80	24	82	32	92	38	76	29	82	39	73	62	51	71	-	95	23	81	52	48
sorbing	η <sub>2</sub> (%)	10.0	23.3	27.1	9.2	19.6	10.1	13.4	20.5	22.9	15.5	24.8	22.3	17.0	27.0	30.1	19.8	27.2	13.5	22.6	25.7	20.9	21.4	24.6	19.7	23.3	30.1	50.2	19.5	34.3	14.4	21.7	36.5
2 <sup>13-8</sup> ): ab	(%) 1μ	76.3	46.6	32.5	69.69	47.1	66.7	49.4	79.3	80.8	47.3	19.3	61.8	41.6	27.4	64.7	16.1	68.3	31.7	28.4	27.8	33.1	60.8	71.5	31.2	22.8	58.2	0.3	42.7	17.7	50.5	23.5	21.6
Design 1 (	η <sub>abs, net</sub> (%)	10.2	23.3	27.2	9.4	19.7	10.2	13.6	20.5	23.0	15.6	24.8	22.5	17.1	27.1	30.2	19.9	27.1	13.6	22.5	25.7	20.9	21.5	24.7	20.0	23.5	30.1	50.4	19.6	34.4	14.5	22.0	36.7
esults for I	η/η <sub>max, C</sub> (%)	58.2	41.4	24.5	67.8	25.2	72.1	52.1	61.2	68.2	58.8	55.0	36.8	77.8	20.1	74.2	25.6	70.7	34.4	72.3	19.2	77.3	34.2	65.8	50.2	42.8	6.99	0.5	92.2	17.4	78.5	41.3	31.7
e D.7: Ro	(%) 1	7.6	10.9	8.8	6.4	9.2	6.7	6.6	16.3	18.5	7.3	4.8	13.8	7.1	7.4	19.4	3.2	18.6	4.3	6.4	7.1	6.9	13.0	17.6	6.2	5.3	17.5	0.2	8.3	6.1	7.3	5.1	7.9
Table	$r_{cav}$ (cm)	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2	9.1	15.2	15.2	9.1	15.2	9.1	9.1	15.2
	$r_i$ (cm)	0.58	0.58	0.97	0.32	0.97	0.35	0.58	0.54	0.97	0.97	1.62	0.54	1.62	0.58	0.97	0.90	0.97	0.97	1.62	0.54	1.62	0.58	0.97	0.90	1.62	1.62	2.70	0.90	2.70	0.97	1.62	1.50
	$C_{feed}$ (g/min)	2	9	9	7	9	7	7	9	9	7	7	9	7	9	9	7	9	7	7	9	7	9	9	7	2	9	9	7	9	7	0	9
	$Q_{s}^{(kW)}$	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0	4.8	4.8	7.0	4.8	7.0	4.8	7.0	4.8	7.0
	Ν	з	5	5	6	ε	5	5	6	Э	5	5	6	e	5	5	6	e	5	S	6	Э	5	5	6	ю	S	S	6	e	5	S	6
	Design	1	7	З	4	5	9	7	8	6	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32

	r								1							_					
$\max_{(kW/m^2)} q_{abs,s}$	957	752	919	1012	947	1026	993	783	1044	863	853	934	932	946	1088	912		$\bigcirc$	000000	9	
$T_{min}$ (K)	1965	1847	1803	1888	1897	1987	1921	1762	1990	1919	1732	1834	1843	1960	1855	1/40	00		00		
$T_{max}$ (K)	2019	2000	2027	2145	2036	2023	2038	1992	2066	2027	2003	2024	1967	2036	2085	2019	000		680	) tî	avity
$\begin{array}{c} X_{avg} \\ (\%) \end{array}$	55	62	75	45	75	39	65	70	75	LL	78	67	74	65	78	8/	0 0 0 0	ω	80%	2	bsorbing c
X <sub>max</sub> (%)	57	67	81	49	76	44	99	75	LL	81	84	72	75	67	80	82					2 <sup>6-2</sup> ): al
$\eta_2^{(\%)}$	18.8	20.6	24.0	16.5	22.9	16.5	20.9	22.5	22.9	24.7	30.1	22.7	27.7	21.7	25.2	28.0	0	- Cu	6	0	esign 2 (
(%) 1μ	80.2	84.1	84.9	76.6	88.8	65.1	84.6	84.6	89.4	85.8	69.5	80.7	78.6	83.1	84.1 77.1	1.6/	<u> </u>		$\sqrt{0}$		s for D
η <sub>abs, net</sub> (%)	18.9	20.7	24.0	16.6	22.9	16.6	21.0	22.6	23.0	24.9	30.2	22.8	27.9	21.8	25.4	7.87			000	5	figuration
$\eta/\eta_{max,C}^{(\%)}$	55.4	62.5	75.4	45.1	74.7	38.9	64.8	66.69	74.9	77.5	78.4	66.8	73.6	65.5	78.1	/8.1				$\leq$	ube con
(%) u	15.1	17.4	20.4	12.6	20.3	10.7	17.7	19.0	20.4	21.2	20.9	18.3	21.8	18.0	21.2	21.1		$)^{\omega}$		)=	tre D.6: T
$f_r$	1	1	1	1	2.5	2.5	2.5	2.5	Э	С	С	С	2.5	2.5	2.5	<b>C</b> .2		$\langle$		$\leq$	Figu
Outer $r_t$ (cm)	0.58	0.58	0.97	0.32	0.81	0.31	0.52	0.51	0.97	0.97	1.62	0.54	1.35	0.52	0.87	0.84	0 0 0 0	~	00000	þ	
N	3	5	ε	5	5	6	5	6	3	5	С	5	5	6	ŝ	h					
Design	1	2	б	4	5	9	7	8	6	10	11	12	13	14	15	10	0 0 0	)-	000	Do	

Table D.8: Results for Design 2  $(2^{62})$ : absorbing cavity

 absorbing cavity
composite):
face-centered central
Table D.9: Results for Design 3 (

$\max_{(kW/m^2)} a_{bs,s}$	738	642	802	686	371	300	433	321	738	642	802	686	371	300	433	321	642	509	527	568	809	387	464	619	541	541	541
${T_{min} \over ({ m K})}$	1614	1638	1724	1373	1585	1297	1446	1427	1947	1589	1737	1756	1603	1663	1652	1406	1639	1455	1528	1461	1579	1416	1417	1551	1615	1412	1485
$T_{max}$ (K)	1742	1862	1879	1722	1663	1531	1590	1635	2058	1866	1929	2048	1701	1846	1783	1668	1779	1740	1745	1757	1858	1655	1677	1823	1840	1706	1753
$\stackrel{X_{avg}}{(0\%)}$	16.0	53.5	70.2	15.5	57.6	14.4	10.8	51.1	88.8	23.0	38.0	84.7	34.4	82.6	66.0	34.0	48.0	42.8	44.4	47.6	44.9	42.8	34.4	59.3	77.2	26.7	47.3
$X_{max}$ (%)	20.0	62.3	75.5	27.9	62.5	22.9	12.3	65.2	91.3	31.5	44.1	91.3	39.0	87.8	6.69	51.3	54.6	56.7	53.9	61.5	56.1	54.7	46.6	70.7	84.3	38.7	59.6
$\eta_2^{(\%)}$	51.3	30.5	38.0	51.8	40.6	50.4	53.8	41.6	32.8	47.5	53.7	32.8	53.4	35.5	48.1	54.0	49.1	46.0	46.0	49.2	45.8	48.6	47.0	48.1	38.0	53.0	47.8
(%) 1μ	34.1	71.7	72.4	33.8	54.4	31.7	21.2	47.0	85.6	43.1	60.2	82.0	54.2	72.2	40.0	53.5	63.8	63.1	65.2	63.7	66.5	57.5	55.3	72.7	70.2	48.8	65.5
$\eta_{abs, net}$ (%)	51.4	30.5	38.2	51.8	40.7	50.4	53.9	41.7	32.8	47.5	53.7	32.8	53.4	35.5	48.2	54.0	49.1	46.0	46.0	49.2	45.8	48.6	47.1	48.1	38.0	53.0	47.8
$\eta/\eta_{max,C}$ (%)	16.0	53.7	70.2	15.7	57.6	14.5	10.8	51.3	88.9	23.2	38.0	84.8	34.4	82.7	66.0	34.2	48.1	43.0	44.5	47.8	45.1	42.9	34.5	59.4	77.3	26.9	47.4
μ (%)	17.5	21.8	27.4	17.5	21.9	15.9	11.4	19.5	27.9	20.3	32.2	26.8	28.9	25.3	19.2	28.8	31.2	29.1	30.0	31.2	30.4	27.9	26.0	34.9	26.6	25.9	31.3
$r_{cav}$ (cm)	9.14	9.14	9.14	9.14	15.24	15.24	15.24	15.24	9.14	9.14	9.14	9.14	15.24	15.24	15.24	15.24	12.19	12.19	12.19	12.19	9.14	15.24	12.19	12.19	12.19	12.19	12.19
$r_t$ (cm)	1.75	0.72	2.39	1.13	3.33	1.52	4.49	2.24	1.75	0.72	2.39	1.13	3.33	1.52	4.49	2.24	3.02	1.41	1.59	2.30	1.33	2.59	1.96	1.96	1.96	1.96	1.96
$\theta_c$	120	120	180	180	120	120	180	180	120	120	180	180	120	120	180	180	150	150	120	180	150	150	150	150	150	150	150
$C_{feed}$ (g/min)	24	8	8	24	8	24	24	8	8	24	24	8	24	8	8	24	16	16	16	16	16	16	16	16	8	24	16
$(k_{W})$	9	9	9	9	9	9	9	9	8	8	8	8	8	8	8	8	7	٢	7	7	٢	7	9	8	7	٢	L
Geom.	1	7	б	4	5	9	7	8	1	2	б	4	5	9	7	8	6	10	11	12	13	14	15	15	15	15	15
Design	1	7	б	4	5	9	7	8	6	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27





## **Appendix E**:

### Predicted errors in temperature measurements

#### E.1 Heat transfer model

Interior tube surface temperatures are measured via type B or type K thermocouple probes inserted from the top of the tube and bent to touch the tube wall. Contact between the tube wall and the thermocouple tip cannot be verified during experimentation. A macroscopic energy balance describing heat transfer to the thermocouple tip is written to approximate measurement error in the likely event that the thermocouple tip does not maintain contact with the solid wall. Three heat transfer modes are considered: (1) radiation exchange between the tip of the thermocouple and the tube wall, (2) conduction along the length of the thermocouple to the cooled base, and (3) convection from the thermocouple to the surrounding fluid phase.

The thermocouple tip is assumed to be positioned within 0.8 mm of the tube wall and all thermocouple probes are assumed to have a uniform diameter of 1.6 mm. Temperature profiles produced by the combined Monte Carlo and computational fluid dynamics model described in Chapter 5 indicate that the highest tube temperature is maintained over a height of at least 0.5 cm. The view factor from the thermocouple tip to this section of the tube wall is estimated by Monte Carlo ray tracing and, for the dimensions listed above, approaches unity. Tube walls are assumed black and, for these simplifications, the net transport of radiative energy to the thermocouple tip is given in equation E.1.

$$Q_{rad} = \varepsilon_{TC} A_{TC} \left( F_{TC-wall} \sigma T_{wall}^4 - \sigma T_{TC}^4 \right)$$
(E.1)

The thermocouple probe is composed of thermocouple wires surrounded by a layer of thermal insulation and covered with a metal sheath. Heat conduction occurs through both the wire and insulation layers and is described by equation E.2.

$$Q_{cond} = \frac{(T_{TC} - T_{base})}{L} \left( k_{wire} A_{c,wire} + k_{ins} A_{c,ins} \right) = \frac{(T_{TC} - T_{base})}{L} \left[ \pi r_{wire}^{2} \left( k_{wire} - k_{ins} \right) + \pi r_{probe}^{2} k_{ins} \right]$$
(E.2)

Convective heat transfer from the fluid flowing over the bent end of the thermocouple probe is described by equation E.3.

$$Q_{conv} = hA_{TC} \left( T_{TC} - T_{fluid} \right)$$
(E.3)

The convective heat transfer coefficient is calculated from equation E.4 using the mean Nusselt number in equation E.5 derived from an empirical correlation for a cylinder in cross flow given by Churchill and Bernstein [1] where all properties are evaluated at the average of the surface and fluid temperatures.

$$h = \frac{k_{fluid} N u}{2r_{probe}} \tag{E.4}$$

$$Nu = 0.3 + \frac{0.62 \operatorname{Re}_{D}^{1/2} \operatorname{Pr}^{1/3}}{\left[1 + \left(\frac{0.4}{\operatorname{Pr}}\right)^{2/3}\right]^{1/4}} \left[1 + \left(\frac{\operatorname{Re}_{D}}{282000}\right)^{5/8}\right]^{4/5}$$
(E.5)

The energy balance is carried out for a length of the thermocouple probe equivalent to the diameter of the probe. The surface area of this section of a cylindrical probe with a hemispherical tip is given in equation E.6.

$$A_{TC} = 4\pi r_{probe}^2 \tag{E.6}$$

The energy balance at the thermocouple tip is given by equation E.7 and the temperature of the thermocouple tip is approximated from solution of equation E.7.

$$Q_{rad} = Q_{cond} + Q_{conv} \tag{E.7}$$
Table E.1 provides base values of all parameters for calculations of temperature measurement errors. All fluid properties are taken to be those for argon gas at the average of the thermocouple and fluid temperatures using the temperature dependent equations provided in Table 5.8.

Parameter	Base value
L	14 cm
$r_{probe}$	0.8 mm
<i>r</i> <sub>wire</sub>	0.1 mm
<i>r</i> <sub>tube</sub>	0.95 cm
$F_{TC-wall}$	0.99
$T_{base}$	300 K
<i>k</i> <sub>ins</sub>	7 W/m/K
$k_{wire}$	70 W/m/K
$\varepsilon_{TC}$	0.75
$\mathcal{V}_{fluid}$	0.5 m/s
T <sub>TC</sub> - T <sub>fluid</sub>	50 K

Table E.1: Base parameters for calculation of thermocouple temperature

Figures E.1 – E.3 illustrate the calculated difference between the thermocouple temperature and wall temperature under various conditions. Radiation exchange between the tube wall and the thermocouple tip render the measurement insensitive to local fluid conditions for wall temperatures greater than roughly 1400 K. Conversely, convective heat transfer with the surrounding fluid phase dominates at low temperatures and thus temperature measurements below roughly 1000 K depend heavily on local fluid conditions. Thus quantitatively accurate measurements at low temperature are contingent on maintaining physical contact between the tube wall and the thermocouple tip whereas the dominance of radiation exchange at high temperature allows for reasonably accurate temperature measurements provided that the separation distance between the thermocouple and the tube wall is minimal. The calculated temperature measurement is more strongly impacted by the thermal conductivity of the

surrounding insulating material than that of the thermocouple wire as a result of the comparatively higher cross sectional area. Lack of physical contact between the thermocouple tip and the tube wall is predicted to produce an error of at least 30-50 K in the temperature measurement at high temperature.



Figure E.1: Calculated difference between wall and thermocouple temperatures as a function of wall temperature, thermocouple emissivity and fluid velocity



Figure E.2: Calculated difference between wall and thermocouple temperatures as a function of wall temperature, fluid velocity, and fluid temperature



Figure E.3: Calculated difference between wall and thermocouple temperatures as a function of wall temperature and thermal conductivity of thermocouple probe

## E.2 Comparison of temperatures measured on-sun with theoretical models

Predicted errors in experimentally measured temperatures shown in Figures 5.30 and 5.32 were derived from variability between replicate experiments and thus only address random error. The predicted discrepancy between thermocouple and tube wall temperatures for the base parameters listed in Table E.1 typically exceeds this random error, particularly at low temperature when measurements are more strongly impacted by a lack of physical contact between the thermocouple and the tube wall. Figures E.4 and E.5 are analogous to Figures 5.30(b) and 5.32(b) and illustrate the modified temperature measurement error predictions calculated from equations E.1-E.7. As separation between the thermocouple and tube wall uniformly lowers the temperature of the thermocouple probe relative to that of the tube wall, the upper bounds of the predicted error are those from the calculations described by equations E.1-E.7 and the lower bounds remain those assessed from variability between replicate experiments. Comparison of Figures E.4 and E.5 with Figures 5.30(b) and 5.32(b) illustrates that the upper

error bound is only notably increased above that predicted from random error at low temperatures.



Figure E.4: Theoretically predicted temperature profiles for SiC tubes compared with experimentally measured values for the center and outer tubes with errors modified to account for separation between the thermocouple junction and the tube wall



Figure E.5: Theoretically predicted temperature profiles for Inconel tubes compared with experimentally measured values for the center and outer tubes with errors modified to account for separation between the thermocouple junction and the tube wall

## Nomenclature

$A_{c,ins}$	cross-sectional area of insulation within thermocouple probe $(m^2)$
$A_{c,wire}$	cross-sectional area of thermocouple wire (m <sup>2</sup> )
$A_{TC}$	surface area of thermocouple tip $(m^2)$
h	convective heat transfer coefficient (W/m <sup>2</sup> /K)
k <sub>fluid</sub>	thermal conductivity of fluid surrounding the thermocouple tip $(W/m/K)$
<i>k</i> <sub>ins</sub>	thermal conductivity of insulation within thermocouple probe (W/m/K)
<i>k<sub>wire</sub></i>	thermal conductivity of thermocouple wire (W/m/K)
L	length between thermocouple tip and cooled based (m)
F <sub>TC-wall</sub>	view factor between thermocouple tip and heated tube wall section
Nu	Nusselt number
Pr	Prandtl number
$Q_{cond}$	energy conducted from the thermocouple tip to the thermocouple base (W)
$Q_{conv}$	energy transferred by convection to the surrounding fluid (W)
$Q_{rad}$	net radiative energy transferred to the thermocouple tip (W)
<i>r<sub>wire</sub></i>	radius of thermocouple wire (m)
r <sub>probe</sub>	radius of thermocouple probe (m)
Re	Reynolds number
T <sub>base</sub>	temperature at thermocouple base (K)
T <sub>fluid</sub>	fluid temperature at thermocouple tip (K)
$T_{TC}$	temperature of thermocouple tip (K)
$T_{wall}$	heated tube wall temperature (K)
€ <sub>TC</sub>	thermocouple emissivity
σ	Stefan-Boltzmann constant $(W/m^2/K^4)$

## References

1. Churchill, S.W. and Bernstein, M., Correlating Equation for Forced-Convection from Gases and Liquids to a Circular-Cylinder in Cross-Flow. *Journal of Heat Transfer-Transactions of the Asme*, 1977. **99**(2): p. 300-306.