Heat Transfer in Wall-Bounded Gas-Solids Flows

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Heat Transfer in Wall-Bounded Gas-Solids Flows

by

Aaron Michael Lattanzi

B.A., University of Washington, 2013

M.S., University of Colorado, 2017

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This thesis entitled:
Heat Transfer in Wall-Bounded Gas-Solids Flows
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has been approved for the Department of Chemical and Biological Engineering

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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.
Despite the remarkable advancements made by modern science, multi-scale problems still pose a significant challenge to the fields of engineering and mathematics. The transport phenomena occurring within a gas-solids flow is a quintessential multi-scale problem. Specifically, the physics occurring at the sub-particle scale is strongly coupled to the macroscopic behavior of many flowing particles. In addition to a fundamental significance, the mathematical description of a particle-laden flow is crucial to the efficient design and operation of many industrial systems. Products from multiphase unit operations encompass (but are not limited to): petroleum, pharmaceuticals, polymers, limestone, and energy. In recent years, solid particles have played a key role in the area of renewable energy. Namely, efficient designs for concentrated solar power plants (CSPs) have been proposed that utilize solid particles as the heat transfer fluid. Particle-based CSPs employ a near black body (NBB) receiver (i.e., granular heat exchanger) to transfer thermal energy from concentrated sunlight to a gas-solids mixture. Generally, concentrated sunlight is irradiated upon the NBB domain walls and the solid particles undergo heat transfer with the hot walls as they flow through the receiver. To assess the feasibility of these new CSP designs, the accurate prediction of wall-to-particle heat transfer is of primary significance. Due to the novelty of solid particle CSPs, the first steps in quantifying wall-to-particle heat transfer have been concerned with convective and conductive mechanisms only (no radiation). As a result, the present work will be concerned with the convective and conductive transport of thermal energy within a wall-bounded gas-solids flow.

The work here begins with an application-based study of the heat transfer within a NBB receiver. The discrete element method (DEM) is employed to simulate a granular heat exchanger whose domain walls are exposed to a constant total heat flux (irradiated sunlight). Current state-of-the-art methods for simulating wall-to-particle heat transfer were implemented within the DEM
framework. Specifically, closures for the direct conduction mechanism occurring between a particle and wall in contact and indirect conduction mechanism occurring between a particle and wall separated by a thin layer of fluid were added to DEM. Furthermore, a new, total heat flux boundary condition was developed to properly describe the NBB geometry. Previous boundary conditions required that a heat flux be specified to each phase and leads to different wall temperatures for each phase. Physically speaking, the total heat flux at the NBB domain wall is what may be approximated (irradiated sunlight) while the partition of the total heat flux amongst the gas and solids phase will vary in space and time according to the local hydrodynamics. A numerical framework for implementing the latter interpretation for a constant, total heat flux boundary condition is derived and verified against DEM simulation of four granular heat exchanger designs.

Simulation of the NBB receiver showed that a majority of the heat transfer to the particles is due to the indirect conduction mechanism. A comparison of the thermal resistances associated with direct and indirect conduction is formulated and it is noted that indirect conduction will dominate for a wide variety of systems. In light of the significance of indirect conduction, the sensitivity of indirect conduction theory to its two theoretical inputs (fluid lens thickness and surface roughness) is assessed for dynamic, multi-particle systems. Analytical techniques commonly employed by kinetic theory are utilized to average indirect conduction theory and quantify a macroscopic heat transfer coefficient. Inputs to indirect conduction theory (fluid lens thickness and surface roughness) are perturbed individually to quantify their effect upon the macroscopic heat transfer coefficient. The analytical sensitivity analysis is found to agree with DEM simulations and shows that indirect conduction is most sensitive to the fluid lens thickness. However, no rigorous means have been established for setting the fluid lens thickness, and thus greater exploration is warranted to test the validity of indirect conduction theory.

In order to rigorously assess indirect conduction theory, the high fidelity direct numerical simulation (DNS) framework must be utilized. A hybrid lattice Boltzmann - random walk code was provided by Professor Xiaolong Yin at the Colorado School of Mines. However, challenges associated with inter-phase heat transfer needed to be corrected before the DNS code could be
utilized to simulate heat transfer in gas-solids flows - e.g., discontinuity in the thermal diffusivity field due to the presence of fluid and particle. The work here details the modifications made to the DNS code and the case studies utilized to verify the new algorithm.

In addition to the modifications made to DNS for inter-phase heat transfer, a fully developed outflow boundary condition required development. For the wall-bounded flows considered in the present work, the fluid velocity at the outflow plane will span orders of magnitude (from the no-slip surface to the free-stream velocity). However, previous considerations given to outflow boundary conditions in the random walk method have been restricted to the completely diffusion-dominated or completed advection-dominated regimes. In the work here, a general method for imposing an outflow boundary condition on the random walk framework is derived. The semi-reflecting barrier is shown to be a general method for achieving an outflow boundary condition in the random walk method and outputs from DNS are verified against boundary layer theory for flow past a hot plate.

Both modifications to the DNS code (inter-phase and outflow) allow for simulation of heat transfer in wall-bounded gas-solids flows. Therefore, indirect conduction theory may be rigorously compared to predictions made by the new DNS framework. In the work here, DNS simulation of flow past a hot plate and static, cold particle is completed. The heat rate outputs from DNS are directly compared to unbounded convection correlations and indirect conduction theory. Indirect conduction theory is found to capture the first-order effects associated with near-wall heat transfer but misidentifies the critical length scale (fluid lens thickness) as being proportional to the particle radius. By contrast, it is observed that the heat transfer enhancement occurring near the hot wall takes place over length scales associated with the thermal boundary layer thickness of the wall. Finally, a novel convection correlation is developed that is valid for the near-wall region, accounts for indirect conduction mechanisms, and asymptotically decays to the unbounded correlation for large particle-wall separation distances.
Dedication

You put those hours in and look at what you get
Nothing that you can hold, but everything that it is

Different day, same struggle
Slow motion as time slips through my knuckles
Nothing beautiful about it, no light at the end of the tunnel
For the people that put their passion before them being comfortable
Raw, unmedicated heart, no substitute
Acknowledgements

I had the privilege of working with many remarkable people over the last four years. Each of them contributed to the present work in many ways and their help cannot be overstated. Dr. Aaron Morris undoubtably provided the foundation for the present work and my earlier contributions (Chapters 2-3). As a postdoctoral researcher in the Hrenya research group, Dr. Morris served as a mentor to me during my first two years of graduate school. Any coding and high performance computing knowledge I have can be traced back to him. Dr. Casey LaMarche and Dr. William Fullmer helped shape many (if not all) of the chapters here. Their candid feedback on my papers contributed to the content and quality of each manuscript. Professor Xiaolong Yin undoubtably made the final pieces of work here (Chapter 4-6) possible. Not only was Professor Yin gracious enough to share his DNS code, he provided me with a wealth of technical knowledge (lattice Boltzmann method and stochastic differential equations) which I otherwise would not have obtained. Finally, many thanks are owed to Professor Christine Hrenya. The present work would not be possible without the funding, guidance, and resources provided by Professor Hrenya. I entered graduate school looking for something. The intellectual challenges and freedoms offered to be by my work with Professor Hrenya gave me what I was looking for and taught me a lot about myself.
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Chapter 1

Introduction

1.1 Motivation

The design and operation of many industrial processes is highly dependent upon the heat transfer occurring within a multiphase flow. Some common examples may be seen in, but not limited to: fluidized reactors [1–6], calciners [7–9], packed beds [10–15], spouted bed dryers [16, 17], and even granular heat exchangers [18–20]. The products resulting from the aforementioned applications vary widely, and encompass commodities such as energy, limestone, petroleum, polymers, and pharmaceuticals. The utilization of solid particles as a heat transfer medium has sparked great interest in passing years (e.g., the granular heat exchangers mentioned above). The need for clean and renewable energy sources has become readily apparent, with the U.S. alone consuming on average $10^{15} \text{ BTU/Yr}$ over the last two decades [21]. To address growing energy needs, the U.S. Department of Energy (DOE) SunShot Initiative has placed an aim on the development of concentrated solar power plants (CSP) that meet a 0.06 \$/kWh target. In an effort to increase CSP efficiency while reducing overall cost, novel designs that utilize solid particles (sand) as the heat transfer fluid have been proposed. The solid sand particles proposed in the new CSP design have the ability to remain inert at elevated temperatures (1000 °C), can store substantial amounts of thermal energy, and are relatively inexpensive. In contrast, previous CSP designs utilized molten salts for the heat transfer fluid which become unstable at (600 °C) and are far less cost effective than the solid sand particles.

The operation and longevity of solid particle CSPs is highly dependent upon the efficiency
of the near black body (NBB) receiver. The NBB is designed to entail a granular heat exchanger which is exposed to concentrated sunlight; see Figure 1.1. The solid particles undergo heat transfer with hot walls (domain boundaries or immersed surfaces) that are exposed to concentrated sunlight. For the case of Fig. 1.1, the concentrated sunlight would be irradiated upon the ends of the circular tubes and the solid particles would heat up as they cascade through the NBB receiver - i.e., the particles undergo heat transfer with the hot immersed tubes. The hot solid particles vacating the NBB receiver serve as a thermal reservoir and subsequently heat steam to run a steam turbine generator, thereby producing electricity.

Figure 1.1: A schematic of the prototype near black boddy (NBB) receiver developed at the National Renewable Energy Laboratory (NREL). The NBB utilizes solid particles as a heat transfer fluid and plays an integral role within the concentrated solar power plant (CSP).

While novel designs for solid particle CSPs show great promise, the description of the heat transfer within the NBB receiver (the cornerstone of the operation) is not trivial. Despite the pervasiveness of gas-solids heat transfer in many relevant industrial applications (e.g., [1-20] above), a fundamental description for the thermal transport occurring within a gas-solids flow still requires further development. Since the thermal source (sunlight) is introduced at the NBB boundary, the heat
transfer occurring between the solid particles and receiver walls is of great significance.

In general, the heat transfer to a particle will be comprised of multiple mechanisms: (i) interphase convection, (ii) direct conduction stemming from the contact of two solids (particle-particle, particle-wall) (PP, PW), (iii) indirect conduction through a thin layer of fluid between two solids (particle-fluid-particle, particle-fluid-wall) (PFP, PFW), and (iv) radiation (RAD); see Figure 1.2.

As prefaced above, the NBB receiver introduces its thermal source at domain walls and/or immersed surfaces, making the heat transfer mechanisms with the wall (convection, PW, PFW, RAD) of primary concern here. Due to the high design temperatures of particle based CSPs (1000 °C), the impact of wall temperature gradients on the NBB structure are of concern. Rather than targeting the upper operating temperature (1000 °C) right away, a more conservative approach was taken. Namely, the heat transfer and wall temperature gradients were assessed at lower operating temperatures (600 K) to gauge the feasibility of different NBB designs. At absolute temperatures below 700 K, the radiative mechanism does not contribute significantly to the overall heat transfer and the relevant mechanisms may be reduced to convection and conduction only \[22\]. Therefore, the
emphasis of this work will be placed on fundamental descriptions for the convective and conductive transport of thermal energy within a \textit{wall-bounded} gas-solids flow.

The present work is computational and theoretical in nature. However, the value of high fidelity experimental work cannot be overstated. Many of the theories developed herein still require rigorous feedback from experimental work, whether that be validation or refute. Furthermore, many classic assumptions are made by computational methods to either close systems of equations or make simulations computationally feasible. While some assumptions have strong physical and mathematic support, others are far more ad hoc. In contrast to simulations, experiments make no assumption about the relevant system physics. The vital observations made by experiments are therefore a gold standard that we as theorists aim to replicate. While no experiments will be detailed here, the present work is a part of a larger project that does involve experiments.

1.2 Modeling Approaches

In order to model the transport phenomena (momentum, heat, mass) that occurs within a gas-solids system, a variety of techniques are commonly employed. The need for different simulation methodologies can be attributed to the presence of many different scales (spatial and/or temporal) within particle-laden flows. In contrast to classic molecular fluids, macroscopic particles dissipate kinetic energy during collisions due to finite deformation and frictional contacts (surface roughness). These unique features of particle interactions (collisions) ultimately lead to extremely complex flow behavior at the macroscopic level. The multi-scale nature of gas-solids flows can thus be traced to the strong coupling between the flow of a collection of particles and the dynamics occurring at the scale of a binary collision. However, resolving the particle level interactions is computationally expensive and not feasible for simulating even lab-scale systems. Therefore, high fidelity frameworks can be used to resolve great detail on small-scale systems or averaged frameworks can be used to resolve less detail on larger-scale systems \cite{23, 24}; see Figure 1.3. Within the present work, a variety of simulation methods will be utilized to model the heat transfer within a CSP NBB receiver, as well as to fundamentally develop new heat transfer closures for gas-solids flows. For this reason, a
A brief overview of all the relevant numerical frameworks is given below while the numerical method employed in each chapter will be explicitly stated.

1.2.1 Direct Numerical Simulation (DNS)

As shown in Fig. 1.3 (a), the direct numerical simulation (DNS) framework resolves discrete particles and treats the gas phase (red lines) as a continuum. Since the gas phase is a classic molecular fluid, the continuum equations of motion are given by the Navier-Stokes equations:

\[
\frac{\partial \rho_g}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}_g) = 0
\]  

(1.1)
\[
\frac{\partial (\rho_g \mathbf{u}_g)}{\partial t} + \nabla \cdot (\rho_g \mathbf{u}_g \mathbf{u}_g) = -\nabla \cdot \bar{\Pi}_g + \rho_g \mathbf{g}
\]  

(1.2)

where \( \rho_g \) is the fluid density, \( \mathbf{u}_g \) is the fluid velocity vector, \( \bar{\Pi}_g = P_g \bar{\mathbf{I}} + \bar{\tau}_g \) is the fluid stress tensor that is comprised of pressure \( (P_g \bar{\mathbf{I}}) \) and viscous \( (\bar{\tau}_g) \) contributions, \( \bar{\mathbf{I}} \) is the identity matrix, and \( \mathbf{g} \) is the gravity vector. For a classic Newtonian fluid, the viscous stress tensor is given by

\[
\bar{\tau}_g = -\mu(\nabla \mathbf{u}_g + \nabla \mathbf{u}_g^T) + (2/3\mu - \lambda)(\nabla \cdot \mathbf{u}_g)\bar{\mathbf{I}},
\]

where \( \mu \) is the dynamic viscosity of the fluid, \( \lambda \) is the bulk viscosity of the fluid, and \( T \) denotes the transpose of the matrix. For an incompressible \( (\rho_g = \text{constant}) \) Newtonian fluid, the governing equations in 1.1 - 1.2 may be simplified dramatically to

\[
\nabla \cdot \mathbf{u}_g = 0
\]

(1.3)

\[
\rho_g \left( \frac{\partial \mathbf{u}_g}{\partial t} + \mathbf{u}_g \cdot (\nabla \mathbf{u}_g) \right) = -\nabla \cdot P_g \bar{\mathbf{I}} + \mu \nabla \cdot (\nabla \mathbf{u}_g) + \rho_g \mathbf{g}.
\]

(1.4)

The analogous balance for the transport of thermal energy takes the form:

\[
\frac{\partial (\rho_g C_{p,g} T_g)}{\partial t} + \nabla \cdot (\rho_g C_{p,g} T_g \mathbf{u}_g) = - (\nabla \cdot \mathbf{q}_g) - (\bar{\tau}_g : \nabla \mathbf{u}_g) - \frac{\partial \ln \rho_g}{\partial \ln T_g} \left( \frac{DP_g}{Dt} \right)
\]

(1.5)

where \( T_g \) is the thermal temperature of the fluid, \( C_{p,g} \) is the fluid specific heat, \( \mathbf{q}_g = -k_g \nabla (T_g) \) is the heat flux vector, and \( k_g \) is the gas thermal conductivity. The terms on the right hand side of the Eq. 1.5 physically correspond to the diffusion of thermal energy, the generation of thermal energy due to shear work, and the work due to thermal expansion, respectively. If the incompressibility constraint is again imposed, the expansion term in Eq. 1.5 (far right) does not contribute to the internal energy balance. In addition, the shear work \((\tau_g : \nabla \mathbf{u}_g)\) in Eq. 1.5 is small for gases and is often neglected. Therefore, the internal energy balance for an incompressible gas simplifies to the familiar advection-diffusion equation

\[
\rho_g C_{p,g} \left( \frac{\partial T_g}{\partial t} + \mathbf{u}_g \cdot (\nabla T_g) \right) = \nabla \cdot (k_g \nabla T_g).
\]

(1.6)
In contrast to the continuum fluid phase, discrete particles are governed by solid body mechanics - i.e., the application of Newton’s second law to each individual particle. The force balance governing the linear and angular momentum of each particle is given by:

\[ \frac{dx_{p,i}}{dt} = u_{p,i} \]  

\[ m_{p,i} \frac{du_{p,i}}{dt} = F_{g,i} + m_{p,i}g \]  

\[ I_{p,i} \frac{d\omega_{p,i}}{dt} = T_{g,i} \]

where \( x_{p,i} \) is the position of particle \( i \), \( u_{p,i} \) is the linear velocity of particle \( i \), \( F_{g,i} \) is the drag force exerted on particle \( i \) by the fluid phase, \( m_{p,i} \) is the mass of particle \( i \), \( I_{p,i} = \frac{2}{5}m_{p,i}R_{p,i} \) is the moment of inertia, \( \omega_{p,i} \) is the angular velocity, and \( T_{g,i} \) is the net torque applied to particle \( i \) by the fluid phase. Note that the force arising from solid-body contact (collisions) is not present in Eqs. 1.8 - 1.9. Commonly, particle collisions are treated via a 'hard-sphere' approach within DNS for increased computational efficiency [25]. The hard-sphere model assumes that particle collisions are binary and instantaneous. Therefore, the hard-sphere method instantly modifies the velocities of colliding particles according to their incoming relative velocities, rather than integrating a contact force in time. As a result, the hard-sphere method is not valid for dense particle flows where collisions are both enduring and multi-particle in nature. Closure for the post collisional particle velocities according to the hard-sphere method may be found in [25, 26]. The details of the hard-sphere method are not given in here since DNS simulation of colliding particles was not completed in this theis. A key feature of DNS is that the fluid flow is resolved down to the smallest scale (e.g., dissipative micro-scale where kinetic energy is converted to thermal energy [27, 28]). The highly resolved fluid field in DNS allows the drag force (\( F_{g,i} \)) and the torque (\( T_{g,i} \)) in Eqs. 1.8 - 1.9 to be
directly computed via integration of the stress tensor over the surface of the particle:

\[ F_{g,i} = \int \Pi_g \cdot n \, dA \tag{1.10} \]

\[ T_{g,i} = \int R_{p,i} n \times (\Pi_g \cdot n) \, dA \tag{1.11} \]

where \( n \) is the unit normal to the particle surface, \( R_{p,i} \) is the radius of the particle, and \( dA \) is the differential area on the surface of the particle. It should be noted that \( \Pi_g \cdot n \) in Eq. \( 1.10 \) corresponds to the local force vector acting upon a differential surface element that is orthogonal to \( n \). The integration performed in Eq. \( 1.10 \) then physically corresponds to calculating net force acting upon the particle. Analogously, the same can be seen in Eq. \( 1.11 \) for the net torque acting upon the particle. For the DNS work considered here, the particles will be held at a constant temperature (Dirichlet boundary condition), and thus, there is no governing equation for the particle temperature. For gas-solids flows, the Biot number is often small and intra-particle temperature gradients may be neglected. Under these circumstances, the governing equation for the particle temperature may simplified to an ordinary differential in time. While spatial and/or temporal gradients in the particle temperature are not considered here, the rate of inter-phase heat transfer \( \dot{q}_{g,i} \) associated with the particle is still of great significance. \( \dot{q}_{g,i} \) is also found via surface integration in DNS

\[ \dot{q}_{g,i} = \int q_g \cdot n \, dA. \tag{1.12} \]

Since DNS employs a numerical grid that is much smaller than a particle, the inter-phase drag (Eqs. \( 1.10 \) - \( 1.11 \)) and convective heat transfer (Eq. \( 1.12 \)) at the particle surface are outputs from a simulation. Thus, DNS yields high-fidelity predictions for the transport within multiphase flows without the need for closures. However, the implementation of a DNS framework for gas-solids flows is not trivial. The continuum fluid equations (Eqs. \( 1.3 \) - \( 1.4 \)) and solid body mechanic equations (Eqs. \( 1.7 \) - \( 1.9 \)) must be solved while the coupling terms (Eqs. \( 1.10 \) - \( 1.12 \)) are computed
on the fly. The computational overhead posed by a DNS framework limits the system sizes to \( O(10^3) \) particles \[29, 30\]. Therefore, DNS provides a wealth of information for small systems and is often utilized to develop closures for the drag force and convective heat transfer, which can then be utilized in less resolved methods (e.g., DEM and TFM).

1.2.2 Discrete Element Method (DEM)

Similar to DNS, the discrete element method (DEM) resolves individual particles and treats the fluid phase as a continuum (Fig. 1.3 (b)). However, rather than resolving the smallest flow scales of the fluid, DEM accounts for the approximate transfer of momentum and thermal energy between the phases. Specifically, a volume averaged Navier-Stokes is utilized for the fluid phase:

\[
\frac{\partial (\epsilon g \rho g)}{\partial t} + \nabla \cdot (\epsilon g \rho g \mathbf{u}_g) = 0 \tag{1.13}
\]

\[
\frac{\partial (\epsilon g \rho g \mathbf{u}_g)}{\partial t} + \nabla \cdot (\epsilon g \rho g \mathbf{u}_g \mathbf{u}_g) = -\epsilon g \nabla \cdot \bar{\Pi}_g - \sum_{i=1}^{n} \beta_{g,s,i}(\mathbf{u}_g - \mathbf{u}_{p,i}) + \epsilon g \rho g \mathbf{g} \tag{1.14}
\]

where \( \epsilon_g \) is the gas volume fraction, \( \beta_{g,s,i} \) is the interphase momentum transfer coefficient for particle \( i \), and \( \sum_{i=1}^{n} \) is completed over all the particles within a fluid numerical cell (see grid in Fig. 1.3 (b)). The internal energy balance is also volume averaged to yield

\[
\frac{\partial (\epsilon g \rho g C_{p,g} T_g)}{\partial t} + \nabla \cdot (\epsilon g \rho g C_{p,g} T_g \mathbf{u}_g) = -\nabla \cdot (\epsilon g \mathbf{q}_g) - \sum_{i=1}^{n} h_{g,s,i}(T_g - T_{p,i}) \tag{1.15}
\]

where \( h_{g,s,i} \) is the inter-phase heat transfer coefficient and \( \sum_{i=1}^{n} \) is again completed over all the particles within a fluid numerical cell.

At this point, the similarity between the volume average continuum equations for the fluid (Eqs. 1.13 - 1.15) and their single phase counterparts (Eqs. 1.1, 1.2, and 1.5) should be noted. Specifically, the volume averaged equations are essentially the single phase equations with the inclusion of the fluid volume fraction \( (\epsilon_g) \) and source terms for the inter-phase momentum \( (\beta_{g,s,i}) \) and heat \( (h_{g,s,i}) \) transfer. The volume averaging applied to the fluid phase allows for the use of a
numerical grid which is large with respect to the particle diameter ($D_p$) (see grid size in Fig. 1.3 (b)). However, since the local fluid velocity and thermal fields are no longer resolved (sub-particle scale), the inter-phase transfer terms ($\beta_{g,s,i}$ and $h_{g,s,i}$) become unknown source terms that require closure - i.e., surface integration cannot be applied to particles in DEM since the fluid flow is captured on a grid much larger than the particle size. Closures for inter-phase drag ($\beta_{g,s,i}$) and convective ($h_{g,s,i}$) heat transfer may be determined from experiments or DNS simulations; see [29–35].

Discrete particles are resolved in DEM (just like DNS), and thus, the solid body mechanical equations still hold for the particles. However, the computational overhead in DEM is significantly reduced from that in DNS (due to the coarse grid utilized for the fluid phase), and thus, the soft-sphere model is commonly employed for particles in the DEM framework - i.e., the normal and tangential contact forces are resolved for multi-particle collisions. The solid body mechanical equations for the soft-sphere method are given by:

$$\frac{dx_{p,i}}{dt} = u_{p,i}$$  \hspace{1cm} (1.16)

$$m_{p,i}\frac{du_{p,i}}{dt} = \sum_j F_{n,ij} + F_{g,i} + m_{p,i}g$$  \hspace{1cm} (1.17)

$$I_{p,i}\frac{d\omega_{p,i}}{dt} = \sum_j T_{ij}$$  \hspace{1cm} (1.18)

where $F_{n,ij}$ is the normal contact force exerted on particle $i$ by solid-body $j$, and $T_{ij}$ is the torque applied to particle $i$ by solid-body $j$ due to frictional contacts. The normal contact forces during a collision ($F_{n,ij}$) are generally treated as a linear-spring dashpot while a Coulombic friction law is utilized for the torque ($T_{ij}$); see [26, 36]. In addition, since the drag force (interphase momentum transfer) is an unknown source term in the continuum fluid equation, it is also an unkown source term.
term in the solid-body equations. The drag force on a particle in the DEM framework is given by

\[ F_{g,i} = -V_{p,i} \nabla P_g + \frac{V_{p,i} \beta_{g,s,i}}{\epsilon_s} (u_g - u_{p,i}) \]  

(1.19)

where \( V_{p,i} \) is the volume of particle \( i \), \( \epsilon_s \) is the solid volume fraction, and \( \beta_{g,s,i} \) is the drag closure utilized in Eq. 1.14. The internal energy balance for a particle, resulting from the inclusion of all of the relevant heat transfer mechanisms (see Fig. 1.2), is given by:

\[ m_{p,i} C_{p,i} \frac{dT_{p,i}}{dt} = \sum_j (\dot{q}_{ij}^{PP} + \dot{q}_{ij}^{PFP} + \dot{q}_{ij}^{RAD}) + \dot{q}_i^{PW} + \dot{q}_i^{PFW} + \dot{q}_i^{RAD} + h_{g,s,i} (T_g - T_{p,i}) \]  

(1.20)

where \( C_{p,i} \) is the specific heat of particle \( i \), \( \dot{q}_{ij} \) is the rate of heat transfer between particle \( i \) and particle \( j \), \( \dot{q}_i \) is the rate of heat transfer between particle \( i \) and a wall, \( h_{g,s,i} \) is the interphase convective heat transfer coefficient utilized in Eq. 1.15, and the superscript (PP, PW, PFP, PFW, RAD) corresponds to the mechanism in Fig. 1.2. The internal energy balance given in Eq. 1.20 is an ordinary differential in time, and thus, an inherent assumption is that the intra-particle temperature gradients are negligible - i.e., the Biot number \( (Bi = \frac{hD_p}{k_p}) \) is small, where \( k_p \) is the thermal conductivity of the particle. A review of the closures for the different heat transfer mechanisms in DEM may be found in [37].

A comparison between DEM and DNS will show that DEM reduces the computational overhead by utilizing a coarse grid for the fluid phase, but does so at the expense of requiring closures (drag, convection, direct conduction, indirect conduction, and radiation). With modern hardware and efficient parallelization, DEM simulations may reach system sizes of \( O(10^7) \) particles. While DEM offers an order-of-magnitude increase in particle count over DNS, it still falls short of common industrial system scales (\( O(10^{12}) \) particles).

**1.2.3 Two-Fluid Model (TFM)**

Rather than tracking each individual particle (position, velocity, temperature, etc.) like in DEM and DNS, TFM treats the solids phase as a continuum. Therefore, volume averaging may
be applied to both the solids and fluid phase continuum equations [38, 39]. With regard to the fluid phase, the volume-averaged Navier-Stokes equations with inter-phase source terms (drag and convection) is again obtained (Eqs. 1.13 - 1.15). On the other hand, the solids phase yields volume-averaged equations that are similar to the Navier-Stokes equations:

\[
\frac{\partial (\epsilon_s \rho_s)}{\partial t} + \nabla \cdot (\epsilon_s \rho_s \mathbf{u}_s) = 0
\] (1.21)

\[
\frac{\partial (\epsilon_s \rho_s \mathbf{u}_s)}{\partial t} + \nabla \cdot (\epsilon_s \rho_s \mathbf{u}_s \mathbf{u}_s) = -\epsilon_s \nabla \cdot \mathbf{\Pi}_s + \sum_{i=1}^{n} \beta_{g,s,i} (\mathbf{u}_g - \mathbf{u}_s) + \epsilon_s \rho_s \mathbf{g}
\] (1.22)

\[
\frac{\partial (\epsilon_s \rho_s C_{p,s} T_s)}{\partial t} + \nabla \cdot (\epsilon_s \rho_s C_{p,s} T_s \mathbf{u}_s) = -\nabla \cdot (\epsilon_s \mathbf{q}_s) + \sum_{i=1}^{n} h_{g,s,i} (T_g - T_s)
\] (1.23)

where all of the variables have remained the same and the \( s \) subscript is utilized to denotes the solids phase. Since a continuum representation is adopted for the solids phase, the solids velocity \((\mathbf{u}_s)\) and temperature \((T_s)\) no longer correspond to a single particle but the average over many particles within a subvolume. Furthermore, closures are now required for the solids stress tensor \((\mathbf{\Pi}_s = P_s \mathbf{I} + \mathbf{\tau}_s)\) and effective conductivity \((k_{s,eff})\) \((\epsilon_s \mathbf{q}_s = \epsilon_s k_{s,eff} \nabla (T_s))\). The departure of particulate rheology from classic fluids generally stems from the dissipative nature of particle collisions (loss of kinetic energy due to deformation and/or friction) and volume exclusion [40, 42]. Despite these differences, successful closure of the stress tensor [43-46] and heat flux vector [47, 48] have been obtained by drawing an analogy with the kinetic theory for nonuniform gases [49-52]. While a remarkable success, the statistical mechanical route to the continuum equations (i.e., Chapman-Enskog or Grad expansion) is not without some simplifying assumptions. Most notably is the simplification of the particle collision process to only encompass binary, instantaneous, and uncorrelated (molecular chaos) collisions [49, 52]. Due to these assumptions, the closures obtained via kinetic theory are not valid for dense (high solids volume fraction) flows where correlated, enduring, multi-particle collisions occur. In addition, experiments have been utilized for developing closures to the solids continuum equations (e.g., the effective thermal conductivity in [53, 54]). However, the empirical
correlations derived from experiments are limited to the cases studied and are not valid for a generic system. Overall, the TFM allows for the simulation of industrial-scale systems but requires the largest number of closures and the techniques utilized to obtain said closures restrict the operating conditions to moderately dense solids flows.

1.3 Dissertation Objectives

While this thesis is concerned with heat transfer in wall-bounded gas-solids flows, the content spans a wide variety of topics and numerical frameworks. Broadly speaking, the present work may be divided up into contributions that are application-based (Chapter 2) and those that are motivated by the application-based results but are more fundamental in nature (Chapters 3-6). The heat transfer within a CSP NBB receiver is simulated via DEM in Chapter 2. The relevant heat transfer mechanisms are implemented within the DEM framework and a new constant heat flux boundary condition is developed to accurately describe the NBB receiver. Furthermore, it is noted that the indirect particle-fluid-wall (PFW) conduction mechanism (Eq. 1.20) dominates the heat transfer within the NBB receiver. Due to the significance of PFW conduction, the sensitivity of indirect conduction to its theoretical inputs is considered in Chapter 3. Indirect conduction theory is found to be most sensitive to the fluid lens thickness (dashed line in Fig 1.2(c)). Traditionally, the fluid lens thickness is set according to heuristic arguments related to the particle radius, and thus, required further investigation. In order to more rigorously assess the validity of indirect conduction theory, DNS must be utilized. A DNS code was provided for this work by Prof. Xiaolong Yin of the Colorado School of Mines. However, the DNS code required modification in order to resolve the heat transfer occurring in a multiphase system. Therefore, Chapters 4 and 5 are concerned with the modifications made to the DNS code and the verification studies conducted to ensure that the numerical framework is properly implemented. In Chapter 6, indirect conduction theory is rigorously compared to the heat rate outputs (Eq. 1.12) from DNS simulation of laminar flow past a hot plate and a static, cold particle. The thermal boundary layer thickness of the wall is found to be the relevant length scale for near-wall heat transfer in lieu of the fluid lens thickness utilized
by indirect conduction theory. The thermal boundary layer thickness is employed to develop a novel Nusselt number compression that is valid for the near-wall region. Finally, some concluding remarks and recommendations for future work are discussed in Chapter 7.

1.3.1 Development and Verification of a Constant Heat Flux Boundary Condition for Gas-Solids Flows (Chapter 2)

Simulation of the NBB receiver was carried out with the DEM framework due to its compromise between computational overhead and simplifying assumptions. Specifically, the NBB receiver is designed to entail dense (high solids volume fraction) flows that promote particle-wall contacts. Under these conditions, the assumptions inherent in kinetic theory are not valid and the TFM closures break down. By contrast, DEM resolves multiple and enduring collisions, and thus, is valid for dense solids flows. The MFIX-DEM software developed by the U.S. National Energy Technology Laboratory (NETL) for multiphase flows was selected to simulate the NBB receiver. However, MFIX-DEM does not have wall-particle heat transfer mechanisms (PW, PFW) implemented within its framework. The PW conduction model of [55, 56] and PFW conduction model of [57] were selected for implementation within the MFIX-DEM source code due to their pervasive use and consistency with current PP and PFP models already present within MFIX-DEM [37]. In addition, the NBB receiver walls can be approximated by a constant heat flux, due to irradiated sunlight. While the total heat flux to the NBB receiver can be approximated (intensity of sunlight), current state-of-the-art methods for multiphase flux boundary conditions require that a flux be specified for each phase. Practically speaking, the heat fluxes to each separate phase should be dictated by the local hydrodynamics, which then dictate the partition of the total flux between each phase. Since no numerical method existed for the latter interpretation, a new, coupled, multiphase heat flux boundary condition was developed and implemented within the MFIX-DEM framework.
1.3.2 Sensitivity of Indirect Conduction to its Theoretical Inputs (Chapter 3)

While Chapter 2 is concerned with the application of wall conduction models (PW, PFW) within DEM (coarse method), Chapter 3 seeks to fundamentally assess the validity and robustness of said models. The PFW conduction mechanism is first identified as the primary mode of heat transfer in the systems considered (Chapter 2). The sensitivity of PFW conduction to its theoretical inputs is computed via analytical methods commonly employed by classic kinetic theory and compared to outputs from DEM simulations. The analytical analysis here highlights the need for a more rigorous interpretation of PFW model inputs (lens thickness) that take into account the length scales associated with the fluid flow. To thoroughly test indirect conduction theory, DNS must be employed.

1.3.3 Extension of lattice Boltzmann - Random Walk Particle Tracking to Multi-phase Systems (Chapter 4)

Before any DNS simulations could be completed, the hybrid lattice Boltzmann - random walk (LBM-RWPT) framework required modification to allow for the simulation of heat transfer in systems with a discontinuous diffusivity field. Previous work in this area has highlighted the tracer phase biasing issue in the RWPT algorithm caused by discontinuous fields - e.g., a particle and fluid with different thermal diffusivities. The few techniques that have been developed for random walks on discontinuous fields may be broadly grouped into the 'reflective barrier' and 'interpolation' methods. The random walk scheme developed here differs from both the reflective barrier and interpolation methods. Here we employ an interfacial tracer balance to ensure that the net tracer flux is zero when the tracer concentrations (temperature) in each phase are equal (consistency with Fourier’s law). By expanding the modulus of the stochastic step within the high diffusivity medium and only allowing a subset of the tracers within the high diffusivity medium to undergo a diffusive displacement, it can be shown that the tracer displacement moments are preserved and the interfacial balance is satisfied. The new LBM-RWPT algorithm is verified against a host of
case studies and is observed to be in agreement with previous numerical studies.

1.3.4 Development of an Outflow Boundary Condition for Random Walk Particle Tracking (Chapter 5)

In addition to the modifications detailed in Chapter 4, an outflow boundary condition for the RWPT method required development. More specifically, a method for enforcing a fully developed outflow boundary in hybrid RWPT methods is proposed in Chapter 5. The hybrid method entails a hydrodynamic solver (LBM in the present work) that recovers the velocity field \( \mathbf{u} \) and the RWPT solver to recover the scalar field (concentration or temperature). A fully-developed boundary condition is characterized by a zero gradient in both the velocity \( \mathbf{u} \) and scalar field \( T \) in the direction of the outward normal to the boundary plane \( \mathbf{n} \) - i.e., \( \frac{\partial \mathbf{u}}{\partial \mathbf{n}} = \mathbf{0} \) and \( \frac{\partial T}{\partial \mathbf{n}} = 0 \). Therefore, the present work establishes a method for imposing \( \frac{\partial T}{\partial \mathbf{n}} = 0 \) on the RWPT method subject to the constraint that \( \frac{\partial \mathbf{u}}{\partial \mathbf{n}} = \mathbf{0} \) has already been achieved by the hydrodynamic solver. An outflow boundary will in general have a nonzero velocity in the direction normal to the wall \( \mathbf{u} \cdot \mathbf{n} \neq 0 \). Since the displacement of tracers contains a deterministic portion \( \mathbf{u}(\mathbf{r}, t)\Delta t \), the average displacement of tracers will be nonzero and in the direction of the local velocity field. Thus, if \( \mathbf{u} \cdot \mathbf{n} > 0 \) at the boundary, then tracers near the boundary will have an average displacement towards the boundary. Under these conditions, it can easily be seen that the classic reflective barrier (impenetrable) will lead to an accumulation of tracers in the near boundary region. To account for the effects of the hydrodynamic boundary \( \frac{\partial \mathbf{u}}{\partial \mathbf{n}} = \mathbf{0} \), a fictitious mirror image of the tracer distribution at the outflow may be considered. The mirror image inherently satisfies the zero gradient criteria for the temperature field and allows the probability of a tracer vacating the domain to be found analytically.

1.3.5 Comparison of Convective and Conductive Closures for Heat Transfer to a Particle in a Laminar Boundary Layer (Chapter 6)

Accurate predictions for the heat transfer occurring within a gas-solids flow is crucial to the design and operation of many relevant industrial operations. While the assessment of heat
transfer in unbounded systems (no walls) is well documented, work with wall-bounded systems is not present within the literature. Particle-scale closures implemented within the DEM framework (convection and indirect conduction) have been largely relied upon to predict near-wall heat transfer coefficients (utilized for NBB reciever in Chapter 2). However, the particle-scale models have not been validated. In Chapter 6 DNS is utilized to rigorously assess the ability of unbounded convection correlations and indirect conduction to capture the heat transfer to a particle in a laminar thermal boundary layer. Furthermore, a convective correlation that considers boundary effects (indirect conduction) is developed. The correlation agrees with DNS simulations and asymptotically decays to the unbounded Nusselt number as the particle-wall separation distance becomes large.
1.4 Chapter 1 Bibliography


2.1 Abstract

Similar to single-phase flows, multiphase systems with a constant heat flux at the wall are common in practice. Unlike single-phase flows, however, the numerical implementation of a constant boundary flux is non-trivial due to the coupling between phases - i.e., the partition of total flux between the phases can vary in space and time. A numerical technique for modeling such a boundary condition is proposed here and verified via simulations of gas-solid flows. While discrete-particle simulations of monodisperse particles are considered here, the technique can be extended to include radiation, polydisperse systems, and/or a continuum representation of the solids phase.

2.2 Introduction

The transfer of thermal energy in a gas-solid mixture is critical to many industrial processes, with modern examples including, but not limited to: rotary kilns 1–3, fluidized beds 4–8, packed beds 9–11, and heat exchangers with granular media as the heat transfer fluid 12. Products resulting from the aforementioned applications vary widely, and encompass commodities such as limestone, petroleum, polymers, and pharmaceuticals. Despite the pervasiveness of multiphase heat transfer, a fundamental description of the underlying physics still requires further development.

Approaches to modeling heat transfer in a gas-solid flow can be classified by their treatment of the solids phase. The discrete element method (DEM) \cite{13,15} involves the tracking of individual particles, while a two-fluid model (TFM) treats the solid phase as a continuum. For both approaches, the vast majority of previous modeling efforts have been limited to constant-temperature boundary conditions \cite{1,5,7,12,16,17}. However, the constant heat flux boundary condition is of considerable practical importance. For example, unit operations involving heat generation from combustion or reactions are more appropriately described by a specified flux at the boundary than a constant temperature. Moreover, the temperature gradients within the wall play an integral role in the evaluation of mechanical stresses and/or selection of construction materials for the given operation. Unfortunately, the representation of a constant flux boundary condition presents challenges for both DEM and TFM frameworks. Specifically, a constant total heat flux is currently achieved by imposing a constant heat flux upon each phase. In practice, however, the total heat flux to the mixture typically remains constant, while the flux to each phase varies in space and/or time. Few attempts to quantify the latter interpretation of a constant heat flux boundary condition have been undertaken \cite{18,19}, and none have been extended to multiphase flows described using the DEM or TFM framework.

In the current work, we propose a new method for imposing a total heat flux boundary condition on multiphase flows. The new boundary condition (BC) is based on an assumption that all phases experience the same local wall temperature and that heat transfer to each phase occurs in parallel. The resulting BC couples the heat flux at the wall for the gas and solid phases, and also allows the heat fluxes to each phase to vary with space and/or time. The general methodology can be adapted for use in discrete-particle or continuum-solid frameworks, but the focus here is on gas-solid flows simulated using computational fluid dynamics - discrete element method (CFD-DEM). Various systems with a specified heat flux imposed the boundary were considered. The accuracy of the new BC was verified by comparing the wall heat flux obtained from simulations with the imposed values. Moreover, the wall heat fluxes of each phase are shown to vary in space and time, while still maintaining the total specified flux - i.e., the heat fluxes of each phase are appropriately
coupled.

2.3 Computational Method

All simulations were performed via MFIX [20–22], an open-source software developed by the U. S. National Energy Technology Laboratory (NETL) for multiphase flows. Specifically, the hydrodynamics and heat transfer of a gas-solids flow were simulated using the computational fluid dynamics and discrete element method (CFD-DEM) framework. The CFD portion treats the fluid phase as a continuum and employs a numerical grid that is much larger than the diameter of a particle. Particles are treated as discrete entities via DEM. Coupling of the continuum and discrete phases in CFD-DEM occurs via interphase transfer of momentum (drag) and heat (convection). The corresponding governing equations are outlined below.

2.3.1 Fluid Phase

The gas phase is treated as a continuum via the following continuity and momentum balances, respectively [23]:

$$\frac{\partial (\epsilon_g \rho_g)}{\partial t} + \nabla \cdot (\epsilon_g \rho_g \mathbf{v}_g) = 0 \quad (2.1)$$

$$\frac{\partial (\epsilon_g \rho_g \mathbf{v}_g)}{\partial t} + \nabla \cdot (\epsilon_g \rho_g \rho_g \mathbf{v}_g) = -\epsilon_g \nabla P_g + \nabla \cdot \tau_g - \sum_{i=1}^{n} \beta_{g,s,i} (\mathbf{v}_g - \mathbf{v}_{p,i}) + \epsilon_g \rho_g \mathbf{g} \quad (2.2)$$

$$\beta_{g,s,i} = \begin{cases} 
150 \frac{(1-\epsilon_g)^2 \mu_g}{\epsilon_g d_{p,i}} + \frac{7(1-\epsilon_g) \rho_g |\mathbf{v}_g - \mathbf{v}_{p,i}|}{4d_{p,i}} & \epsilon_g < 0.8 \\
C_{d} \frac{3(1-\epsilon_g) \rho_g |\mathbf{v}_g - \mathbf{v}_{p,i}|}{4d_{p,i}} \epsilon_g^{-2.65} & \epsilon_g \geq 0.8 
\end{cases} \quad (2.3)$$

where $\epsilon_g$ is the gas fraction, $\rho_g$ is the gas density, $\mathbf{v}_g$ is the gas velocity, $P_g$ is the gas pressure, $\tau_g = \epsilon_g \mu_g [\nabla \mathbf{v}_g + \nabla \mathbf{v}_g^T] + \epsilon_g \lambda_g tr \left( \frac{1}{2} \left[ \nabla \mathbf{v}_g + \nabla \mathbf{v}_g^T \right] \right)$ is the gas-phase stress, $\mu_g$ is the gas dynamic viscosity, $\lambda_g$ is the gas bulk viscosity, $\beta_{g,s,i}$ is the interphase momentum transfer coefficient for particle $i$ [24], $\mathbf{v}_{p,i}$ is the velocity of particle $i$, $n$ is the number of particles within the CFD cell, $d_{p,i}$
is the diameter of particle $i$, $C_d$ is the coefficient of drag, and $\mathbf{g}$ is the gravity vector. The balance for the internal (thermal) energy of the gas is treated in a similar manner:

$$
\frac{\partial (\epsilon_g \rho_g C_{p,g} T_g)}{\partial t} + \nabla \cdot (\epsilon_g \rho_g C_{p,g} \mathbf{v}_g T_g) = -\nabla \cdot (\epsilon_g k_g \nabla T_g) - \sum_{i=1}^{n} h_{g,s,i} (T_g - T_{p,i})
$$

(2.4)

where $C_{p,g}$ is the gas specific heat, $\mathbf{a}_g = (-\epsilon_g k_g \nabla T_g)$ is the heat flux vector, $T_g$ is the (thermal) gas temperature, $k_g$ is the gas thermal conductivity, $h_{g,s,i}$ is the interphase heat transfer coefficient for particle $i$, and $T_{p,i}$ is the temperature of particle $i$.

### 2.3.2 Solid Phase

In contrast to the continuum representation of the gas phase, the solid phase is treated as discrete particles via DEM. Particles are modeled using a soft-sphere approach, and thus can undergo multiple, enduring contacts. The time evolution of each particle property takes the form of an initial value problem. Since the time step for numerical integration must be smaller than the duration of a collision [25], the DEM time step is generally orders of magnitude smaller than the continuum time step; i.e., the DEM solver completes many time steps per CFD solver time step.

The force balance resulting from the application of Newton's second law to each particle governs particle motion with time:

$$
m_{p,i} \frac{d(\mathbf{v}_{p,i})}{dt} = \sum_j \mathbf{F}_{i,j} + \mathbf{I}_{g,s} + m_{p,i} \mathbf{g}
$$

(2.5)

$$
\mathbf{I}_{g,s} = -V_{p,i} \nabla P_g + \frac{V_{p,i} \beta_{g,s,i}}{\epsilon_s} (\mathbf{v}_g - \mathbf{v}_{p,i})
$$

(2.6)

where $m_{p,i} = \rho_{p,i} V_{p,i}$ is the mass of particle $i$, $\rho_{p,i}$ is the density of particle $i$, $V_{p,i}$ is the volume of particle $i$, $\mathbf{F}_{i,j}$ is the force resulting from contacts between particle $i$ and solid-body $j$ (particle or wall), and $\mathbf{I}_{g,s}$ is the drag force. The linear-spring-dashpot method is used to describe particle
contacts:

\[ F_{i,j} = -\kappa_n \sigma - \eta_n \gamma_{n,\text{crit}} \frac{d\sigma}{dt} \]  

(2.7)

\[ e = e^{\exp \left( -\frac{\pi \eta_n}{\sqrt{1 - \eta_n^2}} \right)} \quad \gamma_{n,\text{crit}} = 2\sqrt{m_{\text{eff}} \kappa_n} \]  

(2.8)

where \( e \) is the restitution coefficient (0.90), \( \kappa_n \) is the spring constant (2000 N/m), \( \gamma_{n,\text{crit}} \) is the critical damping coefficient (recovered in the limit of perfectly inelastic collisions \( e = 0 \)), \( \eta_n \) is the ratio of the damping coefficient to the critical damping coefficient, and \( \sigma \) is the ”overlap” of particle \( i \) and body \( j \). It should be noted that an artificially soft spring constant is used in this work in order to increase the computational efficiency of the DEM framework. However, artificially soft spring constants have been shown to yield artificially high heat transfer, due to increased contact times and overlap [17]. A means of correcting for the softened spring constant is also given in [17], referred to here as ”area” and ”time correction”, though such corrections are not employed in this work for simplicity. Similarly, friction is neglected in this work, and thus no governing equation for the angular momentum is required. It is important to note that although the inclusion of area and time corrections as well as friction will affect the solids hydrodynamics and heat transfer, but does not impact the implementation or accuracy of the boundary condition developed herein. The qualitative nature of these effects will be discussed further in Results.

With regard to heat transfer, radiation is not considered here and thus conduction and convection are the only relevant heat transfer mechanisms. The conductive mechanisms may be divided into two categories: (1) direct conduction stemming from the contact of two solids (PP, PW) and (2) indirect conduction through the thin layer of fluid between two solids (PFP, PFW). Accordingly, the mechanisms under consideration are: particle-particle (PP) conduction, particle-fluid-particle (PFP) conduction, particle-wall (PW) conduction, particle-fluid-wall (PFW) conduction, and in-
In the context of interphase convection, the internal energy balance of a particle is given by [16]:

\[ m_{p,i} C_{p,i} \frac{dT_{p,i}}{dt} = \sum_j (\dot{q}_{i,j}^{PP} + \dot{q}_{i,j}^{PFP}) + \dot{q}_i^{PW} + \dot{q}_i^{PFW} + h_{g,s,i}(T_g - T_{p,i}) \] (2.9)

where \( C_{p,i} \) is the specific heat of particle \( i \), \( \dot{q}_{i,j} \) is the rate of heat transfer between particle \( i \) and particle \( j \), and \( \dot{q}_i \) is the rate of heat transfer between particle \( i \) and a wall. Note that an inherent assumption of Eq. 2.9 is an isothermal particle or small Biot number \( (Bi << 1) \) (i.e., no spatial temperature gradients within a particle); the methods developed here can also be adapted to non-isothermal particles as developed by [26].

Since the aim of this work is directed at a new boundary condition for use in CFD-DEM simulations, only the mechanisms pertaining to heat transfer with a wall (\( \dot{q}_i^{PW} \) and \( \dot{q}_i^{PFW} \)) will be expounded upon here. Further details on direct conduction [27], indirect conduction [28], and convection [29,30] are available elsewhere, and the closures used for \( \dot{q}_{i,j}^{PP}, \dot{q}_{i,j}^{PFP}, \) and \( h_{g,s,i} \) in this work are identical to those used by [16]. The particle-wall (direct) conduction takes the form [16,27]:

\[ \dot{q}_i^{PW} = h_{pw,i}(T_w - T_{p,i}) = \frac{4k_{p,i}k_w}{k_{p,i} + k_w} R_c(T_w - T_{p,i}) \] (2.10)

where \( h_{pw,i} \) is the particle-wall conduction heat transfer coefficient for particle \( i \), \( k_{p,i} \) is the thermal conductivity of particle \( i \), \( k_w \) is the thermal conductivity of the wall, \( T_w \) is the wall temperature, and \( R_c = \sqrt{d_{p,i}\sigma - \sigma^2} \) is the radius of contact (resulting from overlap of the particle and wall upon collision).

For particle-fluid-wall (indirect) conduction, an adaptation of the static fluid lens model [28] is utilized [16]; see Figure 2.1. The underlying principle of the model is that each particle is surrounded by a static fluid lens, the thickness of which is a fraction of the particle diameter. When this lens (rather than the particle itself) overlaps with a solid body (wall or other particles), one-dimensional conduction through the fluid lens is assumed to occur between the particle and solid body.
In mathematical terms, the closure for particle-fluid-wall conduction takes the form:

$$\dot{q}_{PFW}^{i} \equiv h_{PFW,i}(T_w - T_{p,i}) = \int_{r_{in}}^{r_{out}} 2\pi k_g r \frac{T_w - T_{p,i}}{\max(l, s)} dr$$

(2.11)

$$r_{in} = \begin{cases} r_s = \sqrt{R_p^2 - (s - R_p - \delta)^2} & \delta \leq s \\ 0 & \delta > s \end{cases}$$

$$r_{out} = \begin{cases} \sqrt{R_p^2 - (R_p + \delta)^2} & \delta > \sqrt{R_{Lens}^2 - R_p^2} - R_p \\ R_p & \delta \leq \sqrt{R_{Lens}^2 - R_p^2} - R_p \end{cases}$$

where $h_{PFW,i}$ is the particle-fluid-wall conduction heat transfer coefficient for particle $i$. The lower integration bound ($r_{in}$) in Eq. 2.11 depends on whether the bottom of the particle is within the minimum conduction distance ($s$) of the wall. For the case of a particle-wall separation distance ($\delta$) greater than the minimum conduction distance ($\delta > s$), the lower bound of integration is zero. For the opposite case ($\delta \leq s$), the lower integration bound becomes the radial position ($r_s$) at which the conduction distance ($l$) equals the minimum conduction distance ($s$). A minimum conduction distance is needed in two cases. First, the presence of surface asperities leads to finite separation between the particle and wall. Second, rarefaction effects become non-negligible as the separation distance decreases to the order of magnitude of the mean free path of the gas. These physical justifications for a minimum separation distance also have a mathematical counterpart; namely,
a singularity will develop in the integrand of Eq. 2.11 as the conduction distance \( l \) approaches zero - i.e., solid-body contact. Since the particles are assumed to be perfectly smooth, a minimum conduction distance on the order of magnitude of the mean free path of the gas is employed here \( (s = 2.75 \times 10^{-8} [m]) \). The upper integration bound \( (r_{out}) \) is the intersection point between the fluid lens and wall, and is constrained to be less than the particle radius \( (R_p) \). The thickness of the fluid lens can have a noticeable impact on the solids heat transfer, but does not affect the implementation of the boundary condition. For this reason, the fluid lens thickness utilized in other works \[10, 16\] was adopted here and kept constant \( (R_{Lens} = 1.4R_p) \).

### 2.4 Development of Heat Flux Boundary Condition

When considering heat transfer with a boundary, three classical conditions arise: (1) constant wall temperature (Dirichlet), (2) constant wall flux (Neumann), or (3) a linear combination of types 1 and 2 (Robin). For single-phase systems, the implementation of a constant wall flux (Neumann) boundary condition (BC) into a CFD code is straightforward and well documented. However, the state-of-the-art for extending a Neumann BC to multiphase flows is to specify a constant heat flux to each phase \[21\]. Practically speaking, it is often the total heat flux to the mixture that remains constant, while the fluxes to each phase may vary in space and time. For this more general case of constant total flux to the mixture, we assume here that (i) both the gas and solid phases experience the same wall temperature and (ii) the heat transfer to each phase occurs in parallel. Therefore, the total heat flux at the wall can be written as a sum of the heat fluxes to each phase, which may vary with time and space:

\[
\vec{q}_w = \vec{q}_g(x, t) + \vec{q}_s(x, t) \tag{2.12}
\]

Since Eq. 2.12 couples the gas and solid frameworks (CFD and DEM) at the boundary, special attention is required to close the heat flux terms. More specifically, because the gas phase is treated as a continuum, the solution of its internal energy balance yields a single temperature
for a given numerical (CFD) cell, including the cell adjacent to the wall. Correspondingly, the wall temperature used for the particle heat transfer (Eqs. 2.10, 2.11) is dictated by the CFD cell it resides in (i.e., wall temperature gradients smaller than the CFD cell that may arise from the discrete nature of the particles cannot be resolved within a CFD cell). Therefore, the heat flux to the gas phase and solid phase must be given on a CFD-grid basis. The gas-phase flux $q^n_g$ is already in terms of continuum variables (Eq. 2.4). However, the heat flux to each particle is resolved in DEM (Eqs. 2.10, 2.11) and thus $q^n_s$ is not in terms of a CFD-grid basis a priori. To recast the individual particle fluxes obtained via DEM for implementation in a CFD cell (continuum), the solids flux is taken as the spatial and temporal average of the total particle-wall conduction occurring within a given CFD cell and over a continuum time step:

$$q^n_s(x, t) = \frac{1}{pA_c} \sum_{j=1}^{P} \sum_{i=1}^{n_j} H_{s,i}(T_w - T_{p,i}) = T_w A - B$$ (2.13)

$$A = \sum_{j=1}^{P} \sum_{i=1}^{n_j} \frac{H_{s,i}}{pA_c}, \quad B = \sum_{j=1}^{P} \sum_{i=1}^{n_j} \frac{H_{s,i} T_{p,i}}{pA_c}, \quad H_{s,i} = h_{pw,i} + h_{pfw,i}$$ (2.14)

where $p$ is the number of DEM time steps within a continuum time step, $A_c$ is the area of the CFD cell adjacent to the wall, $n_j$ is the number of particles within a CFD cell adjacent to the wall during the jth DEM time step, $T_w$ is the continuum wall temperature, and $H_{s,i}$ is the total particle-wall heat transfer coefficient for particle $i$. Since the continuum and DEM frameworks are coupled explicitly (i.e., values at the current time step depend on previous time step only), the wall temperature $T_w$ (continuum) in Eq. 2.13 will be constant over all of the DEM iterations associated with a single fluid time step. Substitution of the solids heat flux (Eq. 2.13) and the gas heat flux (Eq. 2.4) for a boundary cell into Eq. 2.12 gives a closed form for the wall flux in a given cell on a CFD (continuum) basis. Spatial discretization of said equation yields the following relations:

$$q^n_w = \epsilon_{g,k-1} k_{g,k-1} \frac{(T_{g,k}^{t+1} - T_{g,k}^{t+1})}{dx_k} + T_{g,k-1}^{t+1} A_t - B^t$$ (2.15)
\[
\frac{(T_{g,k}^{t+1} - T_{g,k-1}^{t+1})}{dx_k} + \frac{A^t}{\epsilon_{g,k-1}^t k_{g,k-1}^t} T_{g,k-1/2}^{t+1} = \frac{q_w^t + B^t}{\epsilon_{g,k-1}^t k_{g,k-1}^t} 
\tag{2.16}
\]

\[
\frac{\partial T_g}{\partial n} + H_w(x,t)T_g = C(x,t) \tag{2.17}
\]

where \( n \) is the outward normal to the boundary, \( k \) refers to the spatial coordinate, \( t + 1 \) is the current time step, \( t \) is the previous time step, \( H_w = A^t/\epsilon_{g,k-1}^t k_{g,k-1}^t \), \( C = (q_w^t + B^t)/\epsilon_{g,k-1}^t k_{g,k-1}^t \), and \( T_{g,k-1/2}^{t+1} = 1/2(T_{g,k}^{t+1} + T_{g,k-1}^{t+1}) \). Inspection of Eq. 2.16 and 2.17 shows that the constant flux BC for the mixture is now formulated as a Robin BC. By contrast, if radiative mechanisms are accounted for, the boundary condition is more naturally formulated as a Dirichlet boundary condition, which depends upon space and time. However, if this approach is taken, the desired root of a fourth order polynomial must be found for each CFD cell at each continuum time step.

The above methodology for implementing a constant wall flux into the CFD-DEM framework can be completed for any number of phases and easily extended to the two-fluid model (solids and gas both treated as a continuum). Finally, since this method involves a distribution of the total wall flux between "M" phases, the dependence upon other phase temperatures (through the B term(s) in Eq. 2.16) can be handled explicitly and there is no need for nonstandard matrices or preconditioning (like in the case of interphase heat transfer) [21, 31].

### 2.5 Systems Simulated

In this work, the thermodynamic properties for the gas phase were treated as functions of thermal temperature while the solids properties were treated as constants. Inputs used for the gas and solid phases are outlined in Table 2.1 and 2.2 respectively.
A total of five different geometries were simulated with the new BC outlined above, as illustrated in Figure 2.2. The first four geometries are falling-particle, vertical heat exchangers with internal baffles. A constant mass inflow of gas and solids was imposed at the top of the heat exchangers and a constant, positive heat flux at the wall (into domain) was imposed upon all side walls. The vertical heat exchangers exhibit two distinct properties that impact the developed BC. First, a transient period exists where the initially empty domain experiences an increase in particle concentration from the mass inflow. The solids heat flux for each CFD cell will be zero until particles enter the cell and undergo conduction with the wall. If the boundary flux is large during this transient period, the solids heat flux will exhibit large gradients in space (like at the leading

<table>
<thead>
<tr>
<th>Table 2.1: Thermal and hydrodynamic fluid properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species: Air</td>
</tr>
<tr>
<td>$\rho_g$ $= \frac{p_g M_w}{RT_g}$</td>
</tr>
<tr>
<td>$M_w = 28.97 \frac{kg}{kmol}$</td>
</tr>
<tr>
<td>$k_g$ $= k_{g,ref} \frac{T_g}{\sqrt{T_{g,ref}}}$</td>
</tr>
<tr>
<td>$k_{g,ref} = 0.0252 \frac{W}{m K}$ $T_{g,ref} = 300 K$</td>
</tr>
<tr>
<td>$C_{p,g}$ $= 1004.2 \frac{J}{kg K}$</td>
</tr>
<tr>
<td>$\mu_g$ $= \mu_{g,ref} \left( \frac{T_g}{T_{g,ref}} \right)^{\frac{3}{2}} \left( \frac{T_{g,ref} + s}{T_g + s} \right)$</td>
</tr>
<tr>
<td>$\mu_{g,ref} = 1.72 \times 10^{-5} Pa s$ $S = 110.4 K$ $T_{g,ref} = 300 K$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 2.2: Thermal and hydrodynamic solid properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>Species: Sand (SiO₂)</td>
</tr>
<tr>
<td>$\rho_{p,i}$ $= 2582 \frac{kg}{m^3}$</td>
</tr>
<tr>
<td>$k_{p,i}$ $= 1.402 \frac{W}{m K}$</td>
</tr>
<tr>
<td>$C_{p,i}$ $= 794.96 \frac{J}{kg K}$</td>
</tr>
<tr>
<td>$d_{p,i}$ $= 200 \mu m$</td>
</tr>
</tbody>
</table>
edge of the solids flow) and time, leading to numerical instabilities; to mitigate this, the wall heat flux was ramped linearly from 0 to 4200 \([W/m^2]\) over a time of 0.5 \([s]\). Second, the system eventually reaches a statistical steady state. Explicit phase coupling by CFD-DEM requires that the "A" and "B" terms in the BC (Eq. 2.16) come from the previous DEM iteration. A physical interpretation of the explicit coupling is that the solids heat flux at the current time step is approximated by that at the previous time step; at steady state, this approximation should be sufficiently accurate. The fifth simulation geometry, however, is a bubbling-bed heat exchanger with a constant positive wall flux imposed upon all side walls. In contrast to the falling-particle heat exchangers, the bubbling bed does not reach a stable steady state due to the presence of bubbling instabilities. Accordingly, the solids-phase heat flux at the wall may change dramatically in space and/or time, thereby providing a more stringent test of the explicit approximation used to formulate the new BC. The numerical and geometric inputs for all of the cases are given in Table 2.3 and 2.4.
Figure 2.2: Schematics of vertical, falling-particle heat exchangers (left) and bubbling bed heat exchanger (right).
Table 2.3: Simulation inputs: Geometry and Operating Conditions

<table>
<thead>
<tr>
<th>Configurations 1-4</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Column Height</td>
<td>9 cm</td>
</tr>
<tr>
<td>Column Width</td>
<td>3 cm</td>
</tr>
<tr>
<td>Column Depth</td>
<td>0.65 cm</td>
</tr>
<tr>
<td>Number of Cells</td>
<td>138 X 46 X 10</td>
</tr>
<tr>
<td>Mass Flux</td>
<td>$180 \frac{kg}{m^2 \cdot s}$</td>
</tr>
<tr>
<td>$\varepsilon_s$</td>
<td>0.50</td>
</tr>
<tr>
<td>$T_g/s,\text{inlet}$</td>
<td>300 K</td>
</tr>
<tr>
<td>$P_g,\text{outlet}$</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>$Q_{wall}$</td>
<td>$4200 \frac{W}{m^2}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Configuration 5</th>
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</tr>
</thead>
<tbody>
<tr>
<td>Column Height</td>
<td>2 cm</td>
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<tr>
<td>Column Width</td>
<td>1 cm</td>
</tr>
<tr>
<td>Column Depth</td>
<td>1 cm</td>
</tr>
<tr>
<td>Number of Cells</td>
<td>100 X 50 X 50</td>
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<tr>
<td>$V_g,\text{inlet}$</td>
<td>$35 \frac{cm}{s}$</td>
</tr>
<tr>
<td>$T_g,\text{inlet}$</td>
<td>300 K</td>
</tr>
<tr>
<td>$T_g/s,\text{initial}$</td>
<td>300 K</td>
</tr>
<tr>
<td>$P_g,\text{outlet}$</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>$Q_{wall}$</td>
<td>$4200 \frac{W}{m^2}$</td>
</tr>
</tbody>
</table>
Table 2.4: Dimensions for Falling-Particle Heat Exchanger

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Baffle-Wall Spacing</th>
<th>Baffle-Baffle Spacing</th>
<th>Baffle Angle</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.228 cm</td>
<td>-0.521 cm</td>
<td>45 Deg</td>
</tr>
<tr>
<td>2</td>
<td>0.424 cm</td>
<td>-0.521 cm</td>
<td>45 Deg</td>
</tr>
<tr>
<td>3</td>
<td>0.228 cm</td>
<td>0.783 cm</td>
<td>45 Deg</td>
</tr>
<tr>
<td>4</td>
<td>0.424 cm</td>
<td>0.521 cm</td>
<td>45 Deg</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.228 cm</td>
<td>0.326 cm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Hopper Angle</td>
<td>45 Deg</td>
</tr>
</tbody>
</table>

2.6 Results

To validate the accuracy of the new total flux BC for CFD-DEM, all five configurations were simulated with a prescribed positive (inward) heat flux at the wall. Simulations of the falling-particle heat exchanger configurations, which reach a statistical steady state, are considered first. In Figure 2.3, the resulting gas volume fraction (top row) and wall temperature (bottom row) profiles demonstrate that regions of lower gas volume fraction (higher solids concentration) result in lower wall temperatures, consistent with expectations. In particular, the solids heat transfer coefficient is much larger than the gas heat transfer coefficient when a high number of particle-wall contacts occur, and that particles in this work have the ability to store significantly more energy.
than the fluid \( \rho_{p,i}C_{p,i}/\rho_gC_{p,g} \gg 1 \), so regions of high solids fraction result in cooler walls.

For a more detailed view of the temperature profiles, the data along the right side walls was extracted and plotted in Figure 2.4. The predicted wall temperatures lead to a "hot spot" near the inlet (at large column heights) for all four configurations, which can be attributed to the rapid dilution of solids as they undergo gravitational acceleration prior to the first baffle. Depending upon the baffle-wall spacing, particle buildup will occur at or above the first baffle and correspond to a decrease in wall temperature due to high heat transfer to the solid phase. After the first baffle, the particles again accelerate and generally become more dilute, leading to slight increases in wall temperature down the length of the column. Furthermore, the alternating baffle configuration (far right) yields wall temperatures that are substantially higher than any other baffle configuration, and thus it is the least desirable geometry for maximizing heat transfer.

Since the conduction mechanisms for the solids phase \( \dot{q}^PW_i, \dot{q}^{PFW}_i \) are primarily a function of particle-wall proximity, they are strongly influenced by system hydrodynamics. As noted above, the softened spring constant utilized here will lead to enhanced solids heat transfer. Area and time correction have recently been developed such that artificially-soft particles can still be used to simulate stiffer materials while maintaining physical accuracy \([17]\). Inclusion of such corrections will reduce the level of solids-phase conduction. The reduction in solids heat transfer will ultimately lead to hotter wall temperatures. By contrast, the inclusion of angular momentum would work in direct opposition to area and time correction. More specifically, angular momentum would serve to further dissipate energy during particle-wall collisions, due to frictional contacts now being accounted for. Particle-wall contacts will be more pronounced in the more dissipative system and thus serve to increase heat transfer, resulting in cooler wall temperatures. It is worth noting that the artificially-soft particles (without area and time corrections) and lack of friction simulated here was done for purposes of simplicity only, and such simplifications do not impact the implementation or verification of the new boundary condition.
Figure 2.3: Falling-Particle Heat Exchangers: Gas fraction profiles (top) and wall temperature [K] profiles (bottom) are given for the four configurations at steady state (simulation time = 1s).

Figure 2.4: Falling-Particle Heat Exchangers: Wall temperatures along the right side wall at steady state (simulation time = 1s). Configurations are numbered from left to right in Figure 2.3.
While simulations of the falling-particle heat exchangers show the expected qualitative behavior, a more quantitative assessment of the new BC is necessary. In Figure 2.5, the heat flux data for the first configuration (far left in Figure 2.3) is given in more detail. Specifically, the heat flux at the wall, averaged over the entire right-side wall, is tracked through the simulation and compared to the specified value, which is a linear ramp. The heat flux obtained using the new BC is in excellent agreement with the imposed value. Furthermore, the local heat flux associated with the gas phase and solid phase was extracted along the right side wall at steady state, and is plotted separately in Figure 2.6. The large fluctuation in solids heat flux near the inlet coincides with the spike in wall temperature (Fig. 2.4) and is due to reduced particle-wall contacts in a region of high void fractions (Fig. 2.3). Nonetheless, the simulated total wall flux is nearly constant along the column wall though the contribution from each phase varies spatially. A close inspection indicates that the spatial oscillations in the solids heat flux corresponds to baffle positions; these oscillations are out of phase with those of the gas phase, illustrating that the phases are indeed coupled and sum to the imposed value at any given location.

Figure 2.5: Heat Exchanger Configuration 1: Wall flux obtained using the new BC is averaged over the right wall and compared to the imposed wall flux as a function of time.
Figure 2.6: Heat Exchanger Configuration 1: Simulated heat flux data for the wall, solids, and gas along the column height at steady state (simulation time = 1s).

The falling-particle heat exchangers are characterized by a stable steady state that makes the explicit approximation of "A" and "B" terms (Eq. 2.16) in the new BC sufficiently accurate. The bubbling bed, on the other hand, is characterized by bubbling instabilities, which lead to large temporal gradients in the solids heat flux. As a result, the simulation of the bubbling bed demonstrates the impact of hydrodynamic instabilities, and more specifically, large temporal gradients in the solids heat flux on the new BC. This effect is illustrated in Figure 2.7 where the simulated wall flux is averaged over the right side wall and compared to the imposed value for two different CFD time steps. The large, dynamic changes in solids heat transfer make the explicit prediction of the solids heat flux insufficiently accurate for the larger time step; the largest continuum time step ($10^{-4}$ [s]), which corresponds to reaching the desired residual ($10^{-5}$ used in all simulations), yields a maximum error of $\sim 40\%$ for the wall flux. However, the error can be made arbitrarily small by reducing $\Delta t$. For example, reducing the continuum time step by a factor of 2 reduces the maximum error to $\sim 1\%$. As indicated by Figure 2.8, the void fraction and temperature profiles for the bubbling bed again show the expected qualitative behavior. For areas of high solids concentration, the resulting wall temperatures are low.
Figure 2.7: Bubbling Bed Configuration 5: Wall flux obtained using the new BC is averaged over the right wall and compared to the imposed wall flux as a function of time.

Figure 2.8: Bubbling Bed Configuration 5: (left) Simulated void fraction and (right) wall temperature profiles (simulation time = 1s).
2.7 Conclusions

The current state-of-the-art for specifying a total heat flux to the boundary of multiphase flows requires the specification of a heat flux to each phase. By contrast, here we develop a boundary condition for total heat flux to the mixture, which allows the heat flux to each phase to vary in space and/or time. This new BC, targeted at CFD-DEM simulations, was utilized to simulate heat transfer between gas-solids flow and a heated wall in five systems: four falling-particle heat exchangers with different baffle configurations, and one bubbling bed heat exchanger. For the falling-particle cases, which achieve a stable steady state, the simulated wall flux achieves a sufficient degree of accuracy using time steps dictated by the residual for the CFD solver. For the bubbling bed heat-exchanger, which is inherently unstable due to bubbling instabilities, the explicit coupling of CFD-DEM requires that the continuum time step be further reduced for sufficient accuracy.

The new boundary condition is of practical importance since many systems are more accurately described by a flux boundary condition rather than constant temperature. Such a boundary condition allows for wall temperature profiles in time and space to be determined and for potential hot spots to be identified. While only monodisperse particles with no internal temperature gradients and non-radiative mechanisms were explored for the CFD-DEM simulations considered in this work, the extension of the boundary condition to polydisperse CFD-DEM, particles with internal temperature gradients in CFD-DEM, radiative mechanisms, and/or the two-fluid models is possible.

For the falling particle heat-exchangers, the heat flux to the solids phase predominately dictated the corresponding wall temperature. Therefore, the NBB wall temperature gradients, and thus the structural feasibility of the design, is highly predicated on the accuracy of the wall-to-particle heat transfer models. The indirect conduction model was highlighted here due to its significant contribution to the overall heat transfer to the particles. However, the sensitivity of indirect conduction to its theoretical inputs (fluid lens thickness, surface roughness) is not well documented, and thus, their impact on NBB wall temperatures is not known a priori. The content of
Chapter 3 will be devoted to quantifying the sensitivity of indirect conduction (primary mechanism) to its theoretical inputs.
Chapter 2 Bibliography


Indirect Conduction in Gas-Solids Systems: Static vs. Dynamic Effects

3.1 Abstract

Conductive mechanisms play an integral role in the transfer of heat through dense gas-solid systems. In particular, the conduction occurring through a thin layer of fluid between the solids (indirect) can become the primary mode for heat transfer within gas-solid systems. However, attempts to evaluate the effect of surface roughness and fluid lens thickness (theoretical inputs) on indirect conduction have been restricted to static, single-particle cases. By contrast, here we quantify these effects for dynamic, multi-particle systems using a non-dimensional, average heat transfer coefficient that is obtained via techniques commonly employed by classic kinetic theory. Analytical predictions for the impact of theoretical inputs on indirect conduction are compared to outputs from computational fluid dynamics - discrete element method simulations. The analytical predictions are in agreement with simulations and show that indirect conduction in static systems is most sensitive to surface roughness, while dynamic systems are sensitive to the fluid lens thickness.

3.2 Introduction

When considering the heat transfer in a gas-solid flow, the total heat flux will be comprised of contributions from conductive, convective, and radiative mechanisms. However, when thermal temperatures within a system are ≤ 700 K, the radiative mechanism is often neglected since

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it does not significantly contribute to the overall heat transfer \[1, 2\]. Further simplification of the relevant heat transfer mechanisms poses a significant challenge, as the relative contributions from conductive and convective mechanisms cannot be easily gauged. More specifically, since the conductive mechanism is primarily a function of particle-particle (or particle-wall) proximity, the magnitude of the conductive heat transfer coefficient for a generic system is not known a priori, as knowledge of all the particle separation distances would be required. However, some qualitative trends are worth noting. Namely, the average separation distance between particles will reduce as the solids volume fraction increases, causing the conductive mechanism to become more prominent. Furthermore, as the interphase velocity differences decrease, the convective mechanism will contribute less to the overall heat transfer. Thus, conduction will tend to dominate the solids heat transfer within dense and/or slow moving flows. Some practical examples can be seen in, but not limited to: packed beds \[3\], fluidized bed reactors \[4, 5\], and heat exchangers with solid particles as the heat transfer fluid \[6\].

The conduction occurring between two solids is made up of two contributions: (i) direct conduction through the contact area between two solids (particle-particle or particle-wall) and (ii) indirect conduction between two bodies separated by a thin layer of fluid (particle-fluid-particle or particle-fluid-wall). A comparison of the thermal resistances stemming from direct and indirect conduction is given by the dimensionless ratio
$$\beta = \frac{R_p k_g}{R_c k_p}$$
where \(R_p\) is the particle radius, \(k_g\) is the gas thermal conductivity, \(R_c\) is the radius of contact resulting from deformation of two bodies, and \(k_p\) is the particle thermal conductivity. For relatively small contact radii (\(R_c\)) and/or large gas conductivity (\(k_g\)), the thermal resistance associated with direct conduction may be orders of magnitude greater than that of indirect conduction (\(\beta >> 1\)) \[6\]. In such cases, the indirect conduction mechanism dominates. In light of its significance in numerous practical applications \[6, 9\] \[11\], the indirect conduction mechanism will remain the focus of the work here, while detailed accounts of direct conduction \[12, 17\] and convection mechanisms \[18, 21\] are available elsewhere.

Various closures have been proposed for indirect conduction in gas-solid systems \[8, 22, 24\], with differences arising from how the conduction through the interstitial fluid is described; see
Figure 2.1. Namely, the definition adopted for the conduction distance \((l)\) and conduction area (region denoted by red arrows) are the primary parameters which differentiate any two methods. In most cases, the conduction distance and/or conduction area are determined from geometric arguments that depend upon inputs to the theory such as particle roughness. The impact of such input parameters on indirect conduction has not been thoroughly vetted and previous considerations have been restricted to simplified systems. Specifically, the impact of input parameters on particle-fluid-wall conduction was considered for a static, single-particle system by Morris et. al. [7]. They employed the static-fluid-lens model of Rong and Horio [22] to describe indirect particle-fluid-wall conduction. The inputs for the static-fluid-lens model are (i) a fluid lens thickness \((R_{Lens})\) and (ii) minimum conduction distance (surface roughness) \((s)\). For the system considered (static, single-particle), it was concluded that the fluid lens thickness does not significantly impact indirect conduction, but that surface roughness does.

Since the system considered by Morris et al. [7] does not account for dynamic motion or multiple particles, the aforementioned conclusions are not necessarily applicable to a more general system. By contrast, the technique given here accounts for the motion of many particles, and thus, is valid for a broader class of systems. Namely, we propose a method for quantifying the impact of theory inputs (surface roughness and fluid lens thickness) on indirect particle-fluid-wall conduction in dynamic, multi-particle systems. To describe the heat transfer resulting from many particles with varying particle-wall separation distances, an average particle-fluid-wall heat transfer coefficient is utilized here. Evaluation of this heat transfer coefficient is achieved by employing a particle-wall distribution function (analogous to the radial distribution function) in conjunction with the particle-fluid-wall conduction theory. Closure of the particle-wall distribution function is achieved by fitting exponential functions to the distributions extracted from computational fluid dynamics - discrete element method (CFD-DEM) simulations by Morris et al. [7]. Analytical predictions for the percent change in average heat transfer coefficient, resulting from changes in the surface roughness and fluid lens thickness, are compared to outputs from CFD-DEM simulations. The analytical predictions are found to be in agreement with simulation results, but show significant
deviation from prior static, single-particle analysis. Specifically, indirect conduction is found to be most sensitive to the fluid lens thickness in dynamic systems but will be strongly governed by surface roughness in static systems.

3.3 Theory: Particle-Wall Conduction

In this work, we consider the indirect particle-fluid-wall conduction of Rong and Horio [7, 22]. In this theory, each particle is assumed to be surrounded by a static fluid lens (dashed line in Fig. 2.1), the thickness of which is a fraction of the particle diameter. The description of the fluid lens as "static" is guided by two physical reasons. First, the interaction of the no-slip boundary conditions (particle and wall) over small distances (δ) will result in fluid velocities, in the region between the particle and wall, which are dramatically reduced from the free-stream velocity. Second, the fluid density is not a strong function of temperature, and thus, density-driven flow between the particle and wall will be minimal. When the fluid lens overlaps a wall, one-dimensional conduction through the fluid lens is assumed to occur between the particle and wall. The resulting rate of heat transfer is found via integration over the area of overlap between the fluid lens and wall; see Eq. 2.11. To evaluate the integral in Eq. 2.11, a fluid lens radius (R_{Lens}) and minimum conduction distance (s) must be specified. Various fluid lens radii have been considered in previous work and range from 1.2R_p to 1.4R_p [6, 8, 23]. If the upper bound of integration (r_{out}) is not allowed to exceed the particle radius (the largest radial distance at which one-dimensional conduction can occur between the particle and the wall), so that the conduction distance (l) does not become ill defined, then a maximum fluid lens radius may be determined from geometric arguments and is given by \sqrt{2}R_p = 1.41R_p. The minimum conduction distance acts as a lower limit for the conduction distance (l) and is necessary to remove the singularity in Eq. 2.11 as the conduction distance tends to zero (solid body contact). However, the minimum conduction distance also has two physical interpretations. First, large-scale asperities on the surface of a particle (roughness) will result in finite separation distances between a particle and wall even at contact. Second, as the conduction distance becomes very small (less than the mean free path of the gas) rarefaction effects
will become non-negligible. For a perfectly smooth particle and wall, the minimum conduction
distance is set to the mean free path of the gas \((2.75 \times 10^{-8} \text{ m})\) to avoid conduction lengths where
rarefaction effects are significant \([7]\). To reduce the parameter space and cast in a more universal
form, Eq. 2.11 is non-dimensionalized:

\[
\hat{h}_{pfw} \equiv \frac{h_{pfw}}{k_g R_p} = \int_{\hat{r}_{in}}^{\hat{r}_{out}} \frac{2\pi \hat{r}}{(1 + \hat{\delta}) - \sqrt{1 - \hat{r}^2}} d\hat{r}
\]

\[
\hat{r}_{in} = \begin{cases} 
\hat{r}_s = \sqrt{1 - (\hat{s} - 1 - \hat{\delta})^2} & \hat{\delta} \leq \hat{s} \\
0 & \hat{\delta} > \hat{s}
\end{cases}
\]

\[
\hat{r}_{out} = \begin{cases} 
\sqrt{\hat{C}^2 - (1 + \hat{\delta})^2} & \hat{\delta} > \sqrt{\hat{C}^2 - 1 - 1} \\
1 & \hat{\delta} \leq \sqrt{\hat{C}^2 - 1 - 1}
\end{cases}
\]

where \(Var\) denotes normalization by the particle radius, and \(\hat{C} = R_{Lens}/R_p\) is the fluid lens propor-
tionality constant. An analytical solution for \(\hat{h}_{pfw}\), as a function of non-dimensional separation
distance (\(\hat{\delta}\)), can be found through a change of variables and integration by parts:

\[
\hat{h}_{pfw} = 2\pi \left[(1 + \hat{\delta}) \ln \left[\frac{\sqrt{1 - \hat{r}_{out}^2} - (1 + \hat{\delta})}{(1 + \hat{\delta}) - \sqrt{1 - \hat{r}_{in}^2}}\right] + \sqrt{1 - \hat{r}_{out}^2} - \sqrt{1 - \hat{r}_{in}^2}\right]
\]

Inspection of the closure for \(\hat{h}_{pfw}\) (Eq. 3.1) shows that dependence upon gas conductivity \((k_g)\)
and particle size \((R_p)\) have been removed and the input parameters (\(\hat{C}\) and \(\hat{s}\)) are not explicit, but
instead appear implicitly via the bounds of integration (\(\hat{r}_{in}\) and \(\hat{r}_{out}\)). Only the non-dimensional
heat transfer coefficient will be considered here, and thus, any subsequent reference to a heat
transfer coefficient refers to its non-dimensional form (\(\hat{h}_{pfw}\)).
3.4 Theoretical analysis: Static, single particle system

Previous work on the sensitivity of indirect conduction to its input parameters ($\hat{C}$ and $\hat{s}$) has been limited to static, single-particle systems [7] and is summarized here. Given a perfectly smooth particle ($\hat{s} = 1.1 \times 10^{-4}$), $\hat{h}_{pfw}$ is plotted as a function of separation distance for various fluid lens proportionality constants ($\hat{C}$); see Figure 3.1. Note that $\hat{h}_{pfw}$ declines sharply with separation distance and reduces to $\sim 20\%$ of its maximum value when the separation distance is just $\sim 5\%$ of the particle radius ($\hat{\delta} = 0.05$). Since the fluid lens thickness is larger than such small separation distances (proportionality constant $\hat{C} = 1.20 - 1.40$), it was concluded that the majority of the heat transfer is captured and thus $\hat{h}_{pfw}$ is fairly insensitive to the fluid lens thickness (over the aforementioned range). In contrast, it was concluded that $\hat{h}_{pfw}$ exhibits a strong sensitivity to the minimum conduction distance $\hat{s}$. Specifically, recall from Fig. 3.1 (and Eq. 3.1) that the minimum conduction distance affects the lower integration bound ($\hat{r}_m$) for small separation distances ($\hat{\delta} \leq \hat{s}$), which is where the largest heat transfer occurs - i.e., the temperature gradient ($T_w - T_{p,i}$) remains constant but the reduction in conduction distance ($\hat{l}$) yields an increase in the overall driving force ($dT/dx$). Considering the same particle in contact with a wall ($\hat{\delta} = 0$), $\hat{h}_{pfw}|_{\hat{\delta}=0}$ is plotted as a function of minimum conduction distance, and given in Figure 3.1. For increasing minimum conduction distances, $\hat{h}_{pfw}|_{\hat{\delta}=0}$ is observed to decrease significantly. The minimum conduction distances in Fig. 3.1 span multiple orders of magnitude to reflect the impact of this parameter for a wide range of roughness values (from the perfectly smooth limit to particles with large surface asperities). Based on these results for the static single-particle system, it was concluded that indirect conduction is relatively insensitive to the fluid lens thickness but sensitive to the minimum conduction distance.
3.5 Theoretical analysis: Dynamic, multi-particle system

Due to the simplified system considered, the static, single-particle analysis of sensitivity to \( \hat{C} \) and \( \hat{s} \) may not be valid for a generic system. More specifically, since the heat transfer resulting from many particles moving towards and away from a wall is inherently neglected, the static, single-particle analysis offers no means of bridging between the particle-scale heat transfer coefficient \( \hat{h}_{pfw} \) at a fixed separation distance with a corresponding macroscopic heat transfer coefficient - i.e, the particle-fluid-wall heat transfer coefficient resulting from numerous near-wall particles in motion. To relax the assumption of a single particle at a fixed separation distance, averaging techniques are utilized to capture the heat transfer coefficient resulting from many particles with varying separation distances. Namely, following the techniques applied in classic kinetic theory, the average particle-fluid-wall heat transfer coefficient may be found by the weighted integral of Eq.
by the particle-wall distribution function [7]:

\[
\overline{H}_{pfw} = \frac{\int \chi(\delta) \hat{h}_{pfw} d\delta}{\int \chi(\delta) d\delta}
\]  

(3.3)

where \( \overline{H}_{pfw} \) is the average particle-fluid-wall heat transfer coefficient, and \( \chi \) is the particle-wall distribution function in the near-wall vicinity (i.e., \( \delta \leq 0.40 \)). The particle-wall distribution function is analogous to the radial distribution function and physically corresponds to the probability of a particle having a separation distance between \( \delta \) and \( \delta + d\delta \), as illustrated in Figure 3.2.

Figure 3.2: Schematic of the particle-wall distribution function \( \chi \), where the two red particles have been identified as having a separation distance within the differential separation distance.

Unfortunately, the particle-wall distribution function cannot be derived analytically. Therefore, no single function which maps all of the particle-wall distribution dependencies to a probability is known (\( f : \mathbb{R}^n \rightarrow \mathbb{R} \), where \( n \) is the number of variables upon which the particle-wall distribution function depends). However, by assuming that the particle-wall distribution function is primarily a function of solids volume fraction \( (\epsilon_s) \), [7] was able to successfully extract particle-wall distribution functions for various \( \epsilon_s \) via discrete element simulations. While not addressed in the present work or in [7], the particle-wall distribution function may also be a function of friction. The exact dependence of the particle-wall distribution function on friction is unknown, though it is expected to act as an additional source of dissipation and lead to particles having a higher probability of being in the near-wall region. Exponential fits of the particle-wall distribution functions found in
have been used in this work:

\[ \chi_{0.60} = g(\hat{\delta}) \]  \hspace{1cm} (3.4)

\[ \chi_{0.58} = 500e^{-141.34\hat{\delta}} + 1.035\hat{\delta}^2 - 0.411\hat{\delta} + 0.431 \]  \hspace{1cm} (3.5)

\[ \chi_{0.52} = 100e^{-12.071\hat{\delta}} \]  \hspace{1cm} (3.6)

\[ \chi_{0.32} = 16.38e^{-2.511\hat{\delta}} \]  \hspace{1cm} (3.7)

\[ \chi_{\rightarrow 0} = 1 \]  \hspace{1cm} (3.8)

where the subscript on the particle-wall distribution function denotes the solids fraction at which the function is valid (\(\chi_{\epsilon_s}\)), and \(g(\hat{\delta})\) denotes the Dirac-delta function. At this time, it should be noted that: (i) each particle wall distribution function is only valid at the solids fraction given in its subscript and (ii) Eqs. 3.5 - 3.7 are direct fits to the data in [7] (see Figure 3.3), but Eqs. 3.4 and 3.8 are taken as limiting bounds to the particle-wall distribution function in the maximum packing and infinitely dilute regimes, respectively. More specifically, all particles are assumed to be in contact with the wall at the maximum solids fraction (taken to be 0.60), and thus, the particle-wall distribution function can be approximated by an impulse at the wall (\(\hat{\delta} = 0\)). By contrast, as the solids fraction tends to zero, it is assumed that all separation distances will be equally likely and the particle-wall distribution function approaches a uniform distribution.
Inserting $\hat{h}_{pfw}$ (Eq. 3.2) and $\chi$ (Eqs. 3.4 - 3.8) into Eq. 3.3 and integrating allows $\bar{H}_{pfw}$ to be found. By further considering the percent change associated with a perturbation to an input parameter, the sensitivity to such changes in input values is more directly evaluated as:

$$%\Delta \bar{H}_{pfw} = 100 \left( \frac{\bar{H}_{pfw,ref} - \bar{H}_{pfw,2}}{\bar{H}_{pfw,ref}} \right) = 100 \left( \frac{\int \chi \left[ h_{pfw,ref} - \hat{h}_{pfw,2} \right] d\delta}{\int \chi \hat{h}_{pfw,ref} d\delta} \right)$$ (3.9)

where $h_{pfw,ref}$ is the particle-fluid-wall closure (Eq. 3.2) with a set of input parameters that maximize heat transfer ($\hat{C}_{ref} = 1.4; \hat{s}_{ref} = 1.1 \times 10^{-4}$), and $h_{pfw,2}$ is the particle-fluid-wall closure (Eq. 3.2) with a different set of input parameters ($\hat{C}_2; \hat{s}_2$). The sensitivity predictions for the dynamic, multi-particle analysis will be in terms of the $%\Delta \bar{H}_{pfw}$ and were found through numerical integration of Eq. 3.9 after perturbing the input parameters ($\hat{C}_2; \hat{s}_2$) away from the reference input parameters ($\hat{C}_{ref}; \hat{s}_{ref}$).

Impact of the fluid lens thickness on indirect conduction, determined via the aforementioned method, is first considered. Sensitivity to the fluid lens thickness is isolated by only perturbing the fluid lens proportionality constant ($\hat{C}_2 = 1.1, 1.2, 1.3$) while keeping the minimum conduction distance equal to the reference state ($\hat{s}_2 = 1.1 \times 10^{-4}$). Before directly evaluating $%\Delta \bar{H}_{pfw}$,
the deviation in single particle heat transfer coefficient \((\hat{h}_{pfw,ref} - \hat{h}_{pfw,2})\), resulting from the perturbation, is considered, and is given in Figure 3.4. For the case of a varying fluid lens thickness, a substantial difference occurs over all separation distances. The cusps in each curve of Fig. 3.4 occur since \(\hat{h}_{pfw,2} = 0\) when the separation distance is greater than the fluid lens thickness \((\hat{\delta} \geq \hat{C}_2 - 1)\); the separation distance at which these cusps occur correspond to the intersections with the x-axis in Fig. 3.1. Integrating the curves in Fig. 3.4 (left) by each particle-wall distribution function yields the \(\%\Delta \bar{H}_{pfw}\) points in Figure 3.4 (right). For the range of fluid lens thicknesses considered, the \(\%\Delta \bar{H}_{pfw}\) is predicted to be non-negligible and increases strongly as the solids fraction decreases.

The observed trend can be traced back to the nature of the particle-wall distribution functions \((\chi_{\epsilon_s})\) and the deviation between two analytical solutions \((\hat{h}_{pfw,ref} - \hat{h}_{pfw,2})\). More specifically, as the solids phase becomes more dilute, the particle-wall distribution functions becomes more uniform and the deviations at larger separation distances become more significant - i.e., particles are more likely to be further away from the wall where non-negligible differences in the single particle heat transfer coefficient occur. By contrast, as the solids fraction becomes large, the particle wall distribution tends toward the delta function and evaluation of Eq. 3.9 approaches a pointwise argument \((\hat{h}_{pfw,ref}\hat{\delta}=0 - \hat{h}_{pfw,2}\hat{\delta}=0)/\hat{h}_{pfw,ref}\hat{\delta}=0\) - i.e., the change in heat transfer coefficient at contact dictates the \(\%\Delta \bar{H}_{pfw}\) because almost all particles are in contact with the wall. Since significant deviations occur over all separation distances (Fig. 3.4 (left)), and not just at contact \((\hat{\delta} = 0)\), the \(\%\Delta \bar{H}_{pfw}\) will increase as the solids fraction approaches the dilute limit.

Therefore, indirect conduction is sensitive to the fluid lens thickness in a dynamic, multi-particle system and the sensitivity will be greater at lower solids fractions.
Figure 3.4: (left) The deviation in single particle heat transfer coefficient, arising from a change in the fluid lens proportionality constant from 1.4 to 1.3, 1.2, and 1.1. (right) The $\% \Delta \bar{H}_{pfw}$, found via Eq. 3.9, arising from a change in the fluid lens proportionality constant from 1.4 to 1.3, 1.2, and 1.1.

The sensitivity of particle-fluid-wall heat transfer to the minimum conduction distance is evaluated in an analogous manner to the fluid lens thickness. Namely, only the minimum conduction distance is perturbed from the reference state ($\hat{C}_2 = 1.4; \hat{s}_2 = 2.2 \times 10^{-4}, 1.1 \times 10^{-3}, 1.1 \times 10^{-2}$).

The deviation in analytical solutions ($\hat{h}_{pfw,ref} - \hat{h}_{pfw,2}$) resulting from this perturbation is given in Figure 3.5 (left). While the maximum deviations are much larger than those observed for a change in fluid lens thickness (Fig. 3.4), the range of separation distances in which a deviation occurs is dramatically reduced (see expanded x-axis of Fig. 3.5 (left)). In contrast to changes in fluid lens thickness, a deviation between heat transfer coefficients only occurs over separation distances less than the larger minimum conduction distance ($\hat{\delta} \leq \hat{s}_2$). Therefore, the integral in Eq. 3.9 will significantly weight zero deviation ($\hat{h}_{pfw,ref} - \hat{h}_{pfw,2}$) unless the particle-wall distribution function is heavily skewed toward small separation distances ($\hat{\delta} \leq \hat{s}_2$). The resulting $\% \Delta \bar{H}_{pfw}$ is illustrated in Figure 3.5 (right). Unlike the fluid lens thickness, indirect conduction is relatively insensitive to the minimum conduction distance, except at high solids fractions. Thus, the dynamic, multiparticle analysis predicts that particle-fluid-wall heat transfer will not be sensitive to the minimum
conduction distance, except for solid fractions near the maximum packing limit.

**Figure 3.5:** (left) The deviation in single particle heat transfer coefficient, arising from a change in the minimum conduction distance from $1.1 \times 10^{-4}$ to $2.2 \times 10^{-4}$, $1.1 \times 10^{-3}$, and $1.1 \times 10^{-2}$. (right) The $\%\Delta \bar{H}_{pfw}$, found via Eq. 3.9, arising from a change in the minimum conduction distance from $1.1 \times 10^{-4}$ to $2.2 \times 10^{-4}$, $1.1 \times 10^{-3}$, and $1.1 \times 10^{-2}$.

### 3.6 CFD-DEM Simulation Methodology

To provide further support for the analytical predictions presented above, a direct comparison between analytical results and computational fluid dynamics - discrete element method (CFD-DEM) simulations is carried out. MFIX [26, 27], an open-source software developed by the National Energy Technology Laboratory (NETL) for multiphase flows, was employed for all simulations (https://mfix.netl.doe.gov/). The fluid phase is treated as a continuum by CFD while discrete particles are resolved in DEM. The governing equations for the fluid phase, solid phase, thermodynamic properties, and DEM collision inputs have been matched to those provided by Morris et al. [7].

Flow down a ramp is selected as the dynamic simulation geometry. Testing the robustness of predictions for fluid lens sensitivity is possible since various solid fractions may be achieved by
simply altering the conditions at the inflow boundary. A schematic of the ramp system is illustrated in Figure 3.6, with simulation conditions given in Table 3.1.

Figure 3.6: Schematic of the ramp simulations, where \( g \) denotes the gravity vector.

Table 3.1: Ramp simulation inputs

<table>
<thead>
<tr>
<th>Geometry and Operating Conditions</th>
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</thead>
<tbody>
<tr>
<td>Column Angle</td>
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<td>Column Width</td>
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<tr>
<td>Column Length</td>
</tr>
<tr>
<td>Number of Cells</td>
</tr>
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<td>Mass Flux (kg/m² s)</td>
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<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>( R_p )</td>
</tr>
<tr>
<td>( T_{g/s,\text{inlet}} )</td>
</tr>
<tr>
<td>( P_{g,\text{outlet}} )</td>
</tr>
<tr>
<td>( T_{\text{wall}} )</td>
</tr>
</tbody>
</table>
A packed bed without fluid flow is chosen as the static simulation geometry, in order to test predictions made for sensitivity to the minimum conduction distance. Specifically, particles will not be moving in the packed bed and the system will be near maximum packing, and thus, the effect of minimum conduction distance will be greatest. A schematic of the packed bed system is illustrated in Figure 3.7 and the simulation conditions are given in Table 3.2.

![Schematic of the packed bed simulations](image)

**Figure 3.7:** Schematic of the packed bed simulations, where \( g \) denotes the gravity vector.

**Table 3.2:** Bed simulation inputs

<table>
<thead>
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<th></th>
</tr>
</thead>
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<tr>
<td>Column Depth</td>
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<td>Number of Cells</td>
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<tr>
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<td>( T_{g/s,initial} )</td>
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</tr>
<tr>
<td>( P_{g,outlet} )</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>( T_{wall} )</td>
<td>400 K</td>
</tr>
</tbody>
</table>
3.7 Results and Discussion

To make direct comparisons between analytical predictions and CFD-DEM simulations, \( \% \Delta \bar{H}_{pfw} \) is extracted from simulations. In particular, simulations were completed with the reference input parameters and a set of slightly perturbed input parameters. The perturbed input parameters were chosen to best represent the spectrum commonly found in other work \([7–9, 25]\):

(i) \( \hat{C}_{ref} = 1.4 \) and \( \hat{s}_{ref} = 1.1 \times 10^{-4} \); \( \hat{C}_2 = 1.2 \) and \( \hat{s}_2 = 1.1 \times 10^{-4} \) and (ii) \( \hat{C}_{ref} = 1.4 \) and \( \hat{s}_{ref} = 1.1 \times 10^{-4} \); \( \hat{C}_2 = 1.4 \) and \( \hat{s}_2 = 1.1 \times 10^{-3} \). The first set of input parameters (set i) corresponds to a change in fluid lens thickness, and the second set of input parameters (set ii) corresponds to a change in the minimum conduction distance. A system-averaged \( \bar{H}_{pfw} \) was obtained from each simulation by first spatially averaging the \( \hat{h}_{pfw} \) values for each numerical wall cell and then time averaging at steady state. Simulations run with each set of input parameters (i and ii) yield two \( \bar{H}_{pfw} \) values and allow the \( \% \Delta \bar{H}_{pfw} \) (i.e., percent deviation from the reference state) to be evaluated. Furthermore, an effective solids fraction was found by the same averaging techniques employed for the \( \bar{H}_{pfw} \).

Simulation results illustrating the sensitivity to static fluid lens thickness have been plotted alongside the analytical predictions for the dynamic, multi-particle analysis; see Figure 3.8 (left). Outputs from CFD-DEM simulations exhibit the same qualitative trends as the analytical prediction. Namely, a reduction in the fluid lens thickness will result in large changes to the \( \bar{H}_{pfw} \) at low solids fractions and small changes at high solids fractions. The inclined ramp simulations (dynamic) reach a \( \% \Delta \bar{H}_{pfw} \) of \( \sim 40\% \) at moderate solids fractions (\( \epsilon_s \approx 20\% \)) but steadily decreases as the solids volume fraction increases. The packed bed simulation (static), which is at a fixed solids fraction (near maximum packing), exhibits a \( \% \Delta \bar{H}_{pfw} \) of only \( \sim 8\% \). Therefore, the fluid lens thickness does significantly affect indirect conduction in dynamic systems, but the impact is attenuated in static systems and/or near the maximum solids fraction. Considering the sensitivity of indirect conduction on minimum conduction distance, simulation results are again compared to analytical predictions; see Figure 3.8 (right). The simulation outputs again show the
same qualitative trends as those predicted by analytical means. Namely, the sensitivity to the minimum conduction distance is opposite of the fluid lens thickness. While particle-fluid-wall heat transfer strongly depends upon the fluid lens thickness at low solids fractions, it is not a strong function of minimum conduction distance, except near the maximum packing limit. The inclined ramp simulations only show a $\%\Delta \bar{H}_{pfw}$ of $\sim 5\%$, but the $\%\Delta \bar{H}_{pfw}$ spikes to $\sim 18\%$ in the packed bed simulation. Thus, the minimum conduction distance is a significant input parameter for static systems but is not a significant input parameter for dynamic systems.

Figure 3.8: (left) The $\%\Delta \bar{H}_{pfw}$, arising from changing the fluid lens proportionality constant from 1.4 to 1.2, found from CFD-DEM simulations of the ramp and packed bed systems alongside the analytical prediction. (right) The $\%\Delta \bar{H}_{pfw}$, arising from changing the minimum conduction distance from $1.1 \times 10^{-4}$ to $1.1 \times 10^{-3}$, found from CFD-DEM simulations of the ramp and packed bed systems alongside the analytical prediction.

While the simulations and analytical predictions exhibit similar qualitative trends, some quantitative deviations between the two exist. Since the $\hat{h}_{pfw}$ utilized for the analytical predictions is identical to the $\hat{h}_{pfw}$ within CFD-DEM, the deviations can be attributed to a mismatch between
the $\chi$ utilized in the theory and the actually $\chi$ present in the simulations. The nature of the deviations suggests that the particle-wall distributions in the present CFD-DEM simulations more heavily weight smaller separation distances than the particle-wall distributions found by Morris et al. [7]. If the particle-wall distributions are more skewed towards contact, the $\%\Delta \bar{H}_{pfw}$ predictions for the fluid lens thickness will decrease (blue line in Fig. 3.8 (left) shifts downward) and the $\%\Delta \bar{H}_{pfw}$ predictions for changes in the minimum conduction distance will increase (blue line in Fig. 3.8 (right) shifts upward). Therefore, differences between analytical predictions and simulation results for both input parameters may be attributed to a single factor. Reasons for the mismatch in the particle-wall distributions may be due to differences in the mass inflow vector between this work and [7]. Namely, the mass inflow vector was aligned with the gravity vector in this work but was orthogonal to the inflow plane in [7]. By aligning the mass inflow vector with the gravity vector the component of the velocity vector normal to the wall is reduced, thereby reducing particle bouncing. Furthermore, [7] notes that $\chi$ displays a small dependence upon the ramp angle and a rotation of the inflow vector can analogously be thought of as an alteration to the angle of inclination in Fig. 3.6. The change to the mass inflow boundary was done to promote convergence and increase computational efficiency.

3.8 Concluding Remarks

An analytical method for assessing the sensitivity of indirect conduction in dynamic systems was proposed. Previous considerations given to model sensitivity were based on a single particle at a fixed location [7]. This static, single-particle analysis indicates that indirect conduction is insensitive to the fluid lens thickness yet sensitive to the minimum conduction distance. Here, we expand upon [7] by accounting for the effects of many particles at varying separation distances in a dynamic system. Trends for model sensitivity, predicted by the new analytical method, exhibit the same behavior as those obtained from CFD-DEM simulations of (dynamic) ramp flow and a (static) packed bed. In particular, the new trends differ considerably from the static, single-particle analysis and suggest a subtler relation between indirect conduction and the model inputs. Namely, the heat
transferred via indirect conduction in a dynamic, multi-particle system is a strong function of the fluid lens thickness, but not a strong function of the minimum conduction distance. By contrast, a static system is strongly dependent upon the minimum conduction distance, but not the fluid lens thickness, consistent with the previous findings of Morris et al. [7].

The sensitivity of the indirect conduction model to physical input parameters is of great practical significance since indirect conduction is a crucial mechanism for heat transfer in dense gas-solid flows. As it stands, significant deviations between heat transfer in experiments and simulations may persist if a poor selection of input parameters is employed. While the minimum conduction distance physically corresponds to surface roughness, and may be experimentally measured [28], no rigorous guidelines for setting the fluid lens thickness exist. Namely, the fluid lens thickness has solely been justified by geometric arguments related to the diameter of the particle. Physically speaking, the thermal and hydrodynamic scales of the fluid may be large or small with respect to the particle and will be a direct function of Reynolds and Prandtl number. In order to more rigorously test the indirect conduction model and fluid lens thickness, the high-fidelity direct numerical simulation framework must be employed. As it stands, the predominant mechanisms for wall-bounded gas-solids flows has an input parameter which is not well defined physically. Therefore, large errors may occur in the prediction of the NBB wall temperatures (i.e., solids heat transfer) that are due to an improper selection for the fluid lens thickness. In Chapter 4 the transition to DNS will take place, courtesy of the code provided by Professor Xiaolong Yin at the Colorado School of Mines. However, the DNS framework must be modified for use in multiphase systems before an exploration on indirect conduction can be completed.
3.9 Chapter 3 Bibliography


Chapter 4


4.1 Abstract

The development of accurate and robust heat transfer correlations for gas-solids flows is integral to the development of efficient multiphase unit operations. Direct numerical simulation (DNS) has been shown to be an effective method for developing such correlations. Specifically, the highly-resolved fields present in DNS may be averaged for use at the macroscopic level. Most commonly, particle-resolved immersed boundary or thermal lattice Boltzmann methods are employed. Here we develop a hybrid DNS framework where the hydrodynamics are resolved by the lattice Boltzmann method and the temperature field by random walk particle tracking (Brownian tracers). The random walk algorithm provides an efficient means for simulating scalar transport and can easily handle complex geometries. However, discontinuous fields pose a significant challenge to the random walk framework - e.g., a particle and fluid with different diffusivities. We derive a technique for handling discontinuities via the diffusivity, arising at a particle-fluid interface, and implement said method within the tracer algorithm. In addition, the heat transfer coefficient in the random walk method is defined and a technique for handling phases with different volumetric heat capacities is also developed. Moreover, the present algorithm is shown to correctly characterize intra-particle temperature gradients present in high Biot number systems. Verification of the code is completed against a host of cases: effective diffusivity of a static gas-solids mixture,

hot sphere in unbounded diffusion, cooling sphere in unbounded diffusion, and uniform flow past a hot sphere. Predictions made by the new code are observed to be in agreement with analytical solutions, numerical solutions, empirical correlations, and previous works.

4.2 Introduction

Fundamentally quantifying the transport phenomena within gas-solids flows often poses a significant challenge, owing to the presence of many different scales within the system (spatial and/or temporal). However, the transfer of thermal energy within a particle-laden flow is a key function of many industrial unit operations: fluidized beds [1–7], packed beds [8–13], spouted bed dryers [14, 15], rotary kilns [16, 18], and granular heat exchangers [19]; and thus, further theoretical advancements in this area are of great practical significance. Particle-resolved, direct numerical simulation (DNS) may be utilized to obtain high-fidelity predictions for the transport phenomena within a particle-laden flow, as the smallest scales present within the system are resolved. While computationally demanding, DNS has emerged as an effective tool for simulating non-isothermal gas-solids flows, as well as quantifying system’s heat transfer coefficients (HTCs) [20–26].

The types of DNS frameworks may be broadly grouped according to the type of numerical grid they employ. Namely, the domain may either be resolved by a body-conforming mesh or the system may be superimposed over a non-conforming grid. Boundary-conforming meshes often utilize integral methods for solution since the complex system geometry is resolved by an unstructured grid - i.e., the Navier-Stokes equations are approximated via finite element and finite volume techniques [27, 28]. Strict enforcement of boundary conditions may be achieved by conforming the numerical grid to the system boundaries. However, if the boundaries are allowed to move, then the domain must be continuously re-meshed, creating a significant computational overhead. By contrast, this overhead is eliminated in methods that use non-conforming grids. For instance, immersed boundary methods (IBMs) do not conform to domain surfaces but instead introduce forcing terms at the boundary nodes to satisfy the desired boundary condition(s) [29, 32]. Alternatively, the domain boundaries may be projected onto a fixed structured grid to generate a grid conforming
approximation of the domain boundaries \[33–35\]. As the boundaries move, the approximation is updated. This update, however, incurs a much lower computational overhead than an unstructured grid.

The lattice Boltzmann method (LBM) is a widely used method for solving the Navier-Stokes equations in particle-laden flows. The concepts and solution procedure for the LBM are founded in the kinetic theory, and as a result, they greatly differ from other frameworks such as finite element, finite difference, and finite volume. Specifically, LBM involves discretization of the continuous Boltzmann equation in a special manner that ensures the recovery of the Navier-Stokes hydrodynamics \[36, 37\]. Thus, LBM involves discrete velocity distribution functions and not the hydrodynamic variables in the Navier-Stokes equations. For this reason, boundary conditions in the LBM framework are easily imposed directly upon the distribution functions.

While the ability of the LBM to efficiently simulate the Navier-Stokes equations is now well documented, the incorporation of scalar transport (thermal energy or concentration) is not trivial. Even though great progress has been made in the area of thermal LBM \[38–41\], the scalar field is still commonly resolved by coupling a secondary framework to the LBM \[42–44\]. Random walk particle tracking (RWPT) is one such framework developed to solve the advection-diffusion equation of a passive scalar. The positions of passive Brownian tracers are tracked as they undergo movements that depend upon the velocity field (advection) and a stochastic term (diffusion). RWPT does not employ any discretization or numerical grid, and thus it is a meshless method which does not suffer from numerical dispersion in advection-dominated flows \[45\]. Furthermore, RWPT is capable of handling non-Fickian transport \[46\], complex geometries \[47, 48\], and is straightforward to parallelize.

Here we expand the hybrid LBM-RWPT framework of \[42, 43\] to allow for the simulation of heat (or mass) transfer in systems with a discontinuous diffusivity field. Previous work in this area has highlighted the significant challenges posed to the RWPT algorithm by discontinuous fields \[47, 49–51\] - e.g., a particle and fluid with different thermal diffusivities. To address the issue of a discontinuous diffusivity field, we derive a method for altering the stochastic (diffusive) movement
of tracers within the higher diffusivity medium such that the correct tracer distribution is achieved at equilibrium (homogenous). Specifically, the modulus of the stochastic step is increased within the high diffusivity medium while only a subset of the tracers within the high diffusivity medium are allowed to undergo a diffusive step. The algorithm developed here is most similar to that of [49], though significant differences occur between the present work and that of [49]. Within the present work and that of [47, 49, 51], the thermal diffusivities associated with the two mediums (gas and solid-particles) are assumed to be constant (but not necessarily equal) and the generation of thermal energy due to shear work is considered negligible. In addition to addressing a discontinuous diffusivity field, in the present work means for quantifying the heat transfer coefficient in the RWPT method is completed and a technique for handling phases with different volumetric heat capacities is developed. The RWPT method developed here is shown to capture the heat transfer occurring in both low and high Biot number \( (Bi = \frac{hD_p}{k_s}) \) systems. Thus, the present method may provide an efficient means for simulating heat transfer in large Biot systems since it does not suffer the computational overhead associated with carrying a highly resolved numerical grid for each particle.

The new hybrid LBM-RWPT code is verified against a variety of systems: effective diffusivity of a static gas-solids mixture, hot sphere in unbounded diffusion, cooling sphere in unbounded diffusion, and uniform flow past a hot sphere. Predictions made by the new code are found to be in agreement with analytical and numerical solutions, as well as previous works [21, 38, 52].

4.3 Numerical Methods

4.3.1 Lattice Boltzmann Method (LBM)

In this work the LBM is employed to resolve the hydrodynamic fields of fluid only - i.e., the density \( (\rho) \) and velocity \( (\mathbf{u}) \) are obtained from the LBM. The algorithm utilized within this work matches that of [33, 34, 53], and thus will only be briefly discussed here. Rather than discretizing the Navier-Stokes equations themselves, LBM involves the discreteization of the continuous Boltzmann equation in time, space, and molecular velocity. As a result, a collection of molecular velocity
distributions (population densities) are stored at each node, for every time step. The discrete velocity distributions are updated through a streaming and collision process:

\[ n_i(r + c_i \Delta t, \Delta t) \equiv n_i^*(r, t) = n_i(r, t) + \Omega_i(n(r, t)) \] (4.1)

where \( n_i \) is the discrete velocity distribution (population density of molecules at position \( r \) with a velocity \( c_i \)), \( \Delta t \) is the LBM time step (scaled to be unity), \( \Omega_i \) is the collision operator, and \( n_i^* \) is the post-collision distribution function. The collision operator in this work is linearized about the local equilibrium state \( (n^eq, q) \) and matches that in [53]. The hydrodynamic quantities may then be found by taking the moments of the discrete distribution functions:

\[ \rho = \sum_i n_i \quad j \equiv \rho u = \sum_i n_i c_i \quad \bar{\Pi} = \sum_i n_i c_i c_i \] (4.2)

where \( j \) is the momentum and \( \bar{\Pi} \) is the fluid stress tensor. Via a Taylor expansion of the finite difference approximation in Eq. 4.1 and completing a Chapman-Enskog expansion, it can be shown that the LBM recovers the Navier-Stokes equations with the following closures for the shear and bulk viscosities [53]:

\[ \eta = -\rho c_s^2 \left[ \frac{1}{\lambda} + \frac{1}{2} \right] \quad \eta_b = -\frac{2\rho c_s^2}{3} \left[ \frac{1}{\lambda_b} + \frac{1}{2} \right] \] (4.3)

where \( \eta \) is the shear viscosity, \( c_s^2 = 1/3 \) is the square of the speed of sound, \( \lambda \) is the eigenvalue of the collision matrix that corresponds to the relaxation of the off diagonal portion of the non-equilibrium stress tensor, \( \eta_b \) is the bulk viscosity, and \( \lambda_b \) is the eigenvalue of the collision matrix that corresponds to the relaxation of the diagonal portion of the non-equilibrium stress tensor. Coupling of the fluid and solids phase is completed by directly imposing a no-slip boundary condition at the particle surface via the link-bounce-back method [53]. The force and torque applied to a given particle is found by accumulating the momentum transfer between fluid and solid at every boundary node. Inter-particle collisions are modeled via the hard sphere approach and thus are binary and instantaneous. Newton’s equation of motion is then employed to find the new velocity (translational
4.3.2 Random Walk Particle Tracking (RWPT)

4.3.2.1 Single Phase Systems

Similar to the LBM, RWPT does not directly involve the advection-diffusion equation. Instead, the positions of many Brownian tracers are monitored as they undergo movement that depends upon the local velocity field and random fluctuations. These tracers can cross the fluid-solid boundary, so the temperature within the fluid and solid particles is tracked in time. From the theory of stochastic differential equations, a connection can be drawn between the distribution of tracer particles and the advection-diffusion equation \[54\]. If an explicit time integration is utilized, the evolution of each tracer position may be generally written as the following \[45, 55\]:

\[
\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + \mathbf{A}(\mathbf{r}_i, t)\Delta t + \mathbf{\xi}(t) \cdot \mathbf{\bar{B}}(\mathbf{r}_i, t)\sqrt{\Delta t}
\] (4.4)

where \(\mathbf{r}_i\) is the position of tracer \(i\), \(\mathbf{A}\) is the drift vector, \(\mathbf{\xi}\) is a random vector whose entries are sampled from a Gaussian distribution with zero mean and unit variance, \(\mathbf{\bar{B}}\) is the diffusive displacement tensor, and \(\Delta t_{RW}\) is the random walk time step. Note that \(\Delta t\) in Eq. \[4.4\] may be set independently of that in Eq. \[4.1\] but should not exceed it. If \(\mathbf{A}\) and \(\mathbf{\bar{B}}\) are chosen in a specific manner, namely

\[
\mathbf{A}(\mathbf{r}_i, t) = \mathbf{u}(\mathbf{r}_i, t), \quad \mathbf{\bar{B}} = \begin{bmatrix}
\sqrt{2\alpha} & 0 & 0 \\
0 & \sqrt{2\alpha} & 0 \\
0 & 0 & \sqrt{2\alpha}
\end{bmatrix}
\] (4.5)

the resulting tracer distribution obeys the Fokker-Planck equation for the advection-diffusion equation with constant diffusivity \[54\]:

\[
\frac{\partial f}{\partial t} = -\nabla \cdot (\mathbf{A} f) + \frac{1}{2} \nabla \nabla : (\mathbf{\bar{B}} \mathbf{\bar{B}}^T f) = -\nabla \cdot (\mathbf{u} f) + \alpha \Delta (f)
\] (4.6)
where \( u(r_i, t) \) is the velocity at the tracer position \( (r_i) \) before the step is completed (found via trilinear interpolation of the LBM velocity field in this work), \( f \) is the tracer density distribution (probability of finding a tracer between \( r \) and \( r + dr \)), \( \overline{B}^T \) is the transpose of the displacement tensor, and \( \alpha \) is the thermal diffusivity. An analogy can then be drawn between the Fokker-Planck equation and the energy equation with constant thermal diffusivity. Namely, if the tracer concentration is taken to be proportional to the thermal temperature, the RWPT method will recover the familiar thermal advection-diffusion equation.

\[
\frac{\partial T}{\partial t} + u \cdot \nabla(T) = \alpha \Delta(T) \tag{4.7}
\]

### 4.3.2.2 Development of Tracer-Based Method for Multiphase Systems

For the case of multiphase systems, the diffusivity may depend upon space \( (\overline{B} = \overline{B}(r)) \) since different phases may have different diffusivities. Under such circumstances, if the drift vector \( (A) \) and displacement tensor \( (\overline{B}) \) are naively chosen to match those in Eq. 4.5, the resulting tracer distribution will not correspond to the macroscopic transport equation - i.e., gradients in the diffusivity field will not be accounted for. If the diffusivity field is smooth, the drift vector may be defined in an alternative manner \( (A \equiv u^* = u + \nabla \cdot \tilde{\alpha}(r)) \) so that the form of the Fokker-Planck equation (Eq. 4.6) is consistent with the advection-diffusion equation (proper macroscopic transport equation is recovered). Due to the dependency upon the gradient of the diffusivity field, the drift velocity \( (u^*) \) may become infinite in a multiphase system - e.g., the diffusivity is discontinuous across a particle-fluid interface. Here we consider the case of a gas-solid mixture in which the thermal diffusivities associated with each phase are not equal and do not have any spatial or temporal dependence. Therefore, a singularity in the drift velocity \( (u^*) \) will be present in the systems considered here and special considerations must be given to ensure the correct macroscopic phenomena is preserved. In the RWPT method, it is most commonly assumed that the diffusivities associated with each phase are equal. However, a few techniques have been developed for random walks on discontinuous fields. The techniques can be broadly grouped into the "reflective barrier"
and "interpolation methods"; see [47, 50, 51]. The random walk scheme developed here differs from both the reflective barrier and interpolation methods and is most analogous to that of [49].

Note that in the present work, as well as [47, 49–51], the interface between two phases yields a discontinuity in the diffusivity field, but the diffusivity within a phase is still assumed to be constant. The approach developed by [49] defines two time scales that are associated with the two phases. The time scales in [49] are related to one another by the ratio of the diffusivities (also assumed constant within a phase in [49]) and the ratio of the tracer concentrations in each phase at equilibrium (referred to as the partition coefficient). Here we employ an interfacial tracer balance to ensure that the net tracer flux is zero when the tracer concentrations in each phase are equal (partition coefficient of 1). An illustrative example as to why the random walk algorithm requires modification can be understood via the simple case of diffusion over a domain with a discontinuous thermal diffusivity - e.g., a solid particle suspended within a fluid. If the system is initialized with a uniform tracer concentration (thermal equilibrium), the tracer concentration should remain homogenous since there are no driving forces (tracer concentration gradients). However, the system will evolve to a state where the concentration of tracers within the high diffusivity medium is less than that of the low diffusivity medium [47] - i.e., equilibrium will be defined by a state where the high diffusivity medium is cooler than the low diffusivity medium and not by a state of equal thermal temperatures. Such behavior is physically incorrect and serves as a basis for how the random walk algorithm should be modified.

By considering the case of steady-state diffusion within a composite medium (Figure 4.1), analytical methods may be employed to determine the appropriate modifications to the random walk framework, such that the proper equilibrium state is restored for the case of unequal diffusivities. The system under consideration is static, and comprised of two materials which have equal temperatures (tracer concentration) and volumetric heat capacities but different thermal diffusivities (conductivities); see Figure 4.1.
Figure 4.1: An illustration of the geometry for steady-state diffusion in a composite medium. The thermal temperature (tracer concentration) and volumetric heat capacity of both materials are equal \( T_1 = T_2 = T, C_{v,1} = C_{v,2} = C_v \), while the diffusivities (conductivities) are not equal \( \alpha_1 \neq \alpha_2, k_1 \neq k_2 \), and yield a discontinuity at the interface (dashed line).

For the case considered, the tracer update (Eq. 4.4) only retains the stochastic term \( r_i(t + \Delta t) = r_i(t) + \xi(t)\sqrt{2\alpha_i \Delta t} \). Therefore, the criteria for a tracer to reach the interface during a step takes the following form:

\[
\xi_x \sqrt{2\alpha_i \Delta t} \geq x'_i
\]

where \( x'_i \) is the separation distance between the current tracer position and the interface, and \( \xi_x \) is the random number sampled in the x-direction. Since the stochastic terms \( \xi_i \) are sampled from a Gaussian distribution, the probability of reaching the interface, for a given separation distance \( x'_i \), can be found by calculating the probability of selecting a value such that Eq. 4.8 is satisfied:

\[
P(x'_i) \equiv \int_{x'_i}^{\infty} \xi_x(\tau) d\tau = \int_{x'_i}^{\infty} \frac{1}{\sqrt{2\pi}} e^{\left(-\frac{x'^2}{2}\right)} d\tau = \frac{1}{2} erfc\left(\frac{x'_i}{2\sqrt{\alpha_i \Delta t}}\right)
\]
where \( P(x'_i) \) is the probability of reaching the interface, and \( \xi_i(\tau) = \frac{1}{\sqrt{2\pi}} e^{-\frac{\tau^2}{2}} \) is the Gaussian distribution from which the stochastic terms are sampled. The probability of reaching the interface \( (P(x'_i)) \) may then be utilized to complete a tracer balance across the interface and over a single time step \((\Delta t)\):

\[
N_t = \int C_1(r) P(x'_1) dV_1 - \int C_2(r) P(x'_2) dV_2
\]

where \( N_t \) is the net number of tracers crossing the interface, \( C_i \) denotes the concentration of tracers in medium \( i \), and \( dV_i \) is the differential volume occupied by medium \( i \). Since the tracer concentration is uniform at steady-state \((C \neq C(r))\), the integrals in Eq. 4.10 may be directly evaluated:

\[
C_i A_c \int_0^{L_i} \frac{1}{2} \text{erfc} \left( \frac{x'_i}{2\sqrt{\alpha_i \Delta t}} \right) dx'_i = C_i A_c \sqrt{\alpha_i \Delta t} \int_0^\infty \text{erfc}(\chi) d\chi = C_i A_c \sqrt{\frac{\alpha_i \Delta t}{\pi}}
\]

\[
\int C_1(r) P(x'_1) dV_1 - \int C_2(r) P(x'_2) dV_2 = \frac{A_c}{\sqrt{\pi}} \left[ C_1 \sqrt{\alpha_1 \Delta t} - C_2 \sqrt{\alpha_2 \Delta t} \right]
\]

where \( A_c \) is the surface area of the interface, \( L_i \) is the system length scale in the direction normal to the interface \((x'_i)\), and \( \chi = \frac{x'_i}{2\sqrt{\alpha_i \Delta t}} \). Since the system length scales are large with respect to the modulus of the diffusive step, the bounds of integration in the middle equality of Eq. 4.11 may be simplified - i.e., as \( x'_i \rightarrow L_i, \chi \rightarrow \infty \). By definition, the net number of tracers crossing the interface should be zero at equilibrium \((N_t = 0)\). By imposing the equilibrium condition upon Eq. 4.12 it can be seen that the tracer concentration (temperature) within each material is not the same unless the diffusivities are equal \((\frac{C_1}{C_2} = \sqrt{\frac{\alpha_2}{\alpha_1}})\). Furthermore, the analytical solution is in agreement with the qualitative behavior previously asserted (tracers will be biased to the lower diffusivity phase at equilibrium).

To rectify the phase biasing issue and restore the proper definition of equilibrium, a twofold approach is taken to modifying the random walk algorithm. First, the displacement matrix \((\bar{B})\) is modified for the higher diffusivity medium \((\alpha_1)\) and a probability of undergoing a diffusive step \((P_{\text{move},i})\) is introduced. Specifically, the magnitude of the displacement matrix is increased for the
higher diffusivity medium while the probability of undergoing a stochastic step within the higher diffusivity medium is reduced; see Eq. 4.13 and 4.14.

\[
B = \begin{cases}
\sqrt{2\frac{\alpha_1}{\alpha_2}} & 0 & 0 \\
0 & \sqrt{2\frac{\alpha_1}{\alpha_2}} & 0 \\
0 & 0 & \sqrt{2\frac{\alpha_1}{\alpha_2}}
\end{cases}
\]

\[P_{\text{move},1} = \frac{\alpha_2}{\alpha_1} \quad P_{\text{move},2} = 1\]  \hspace{1cm} (4.14)

In Eq. 4.13 - 4.14 it has inherently been assumed that \(\alpha_1 > \alpha_2\). Returning to the calculation of the net number of tracers crossing the interface (Eq. 4.12), the requirement of zero net tracer flux at equilibrium (uniform concentration) is satisfied.

\[
\int C_1 P_{\text{move},1} P(x_1')dV_1 - \int C_2 P(x_2')dV_2 = \frac{A_c}{\sqrt{\pi}} \left[ C_1 \frac{\alpha_2}{\alpha_1} \sqrt{\frac{\alpha_1^2}{\alpha_2} \Delta t} - C_2 \sqrt{\alpha_2 \Delta t} \right] = 0 \hspace{1cm} (4.15)
\]

While the appropriate definition for equilibrium is restored, it is not obvious if the modifications will alter the dynamics within the higher diffusivity phase, due to the alteration of the displacement matrix and introduction of the probability of moving. To show that the appropriate macroscopic behavior is retained, the mean squared displacement within the higher diffusivity material is considered:

\[
\langle \Delta r_i^2 \rangle = P_{\text{move},1} \left( \left( \xi_i \sqrt{2\frac{\alpha_1^2}{\alpha_2} \Delta t} \right)^2 \right) = 2 \frac{\alpha_2}{\alpha_1} \frac{\alpha_1^2 \Delta t}{\alpha_2} \langle \xi_i^2 \rangle = 2\alpha_1 \Delta t \hspace{1cm} (4.16)
\]

\[
\langle \xi_i \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tau e^{\left(\frac{-\tau^2}{2}\right)} d\tau = 0 \quad \langle \xi_i^2 \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tau^2 e^{\left(\frac{-\tau^2}{2}\right)} d\tau = 1 \hspace{1cm} (4.17)
\]
where $\langle \cdot \rangle$ denotes an average over all Brownian tracers, $\langle \xi_i \rangle$ is the first moment of the stochastic term, and $\langle \xi_i^2 \rangle$ is the second moment of the stochastic term. The mean squared displacement of tracers within the higher diffusivity material (Eq. 4.16) matches the classic single phase solution \[47\]. Inclusion of these modifications into the RWPT algorithm yields the following update scheme (for $\alpha_1 > \alpha_2$):

$$r_1(t + \Delta t) = r_1(t) + u(r_1, t)\Delta t + \xi(t)\sqrt{2\frac{\alpha_1}{\alpha_2}}\Delta t \left[ 1 - H \left( \zeta - \frac{\alpha_1}{\alpha_2} \right) \right]$$

$$r_2(t + \Delta t) = r_2(t) + u(r_2, t)\Delta t + \xi(t)\sqrt{2\alpha_2}\Delta t$$

where $H$ is the Heaviside function and $\zeta$ is a random number sampled from a uniform distribution on the span $[0, 1]$. The second part of the approach addresses how tracers that reach the interface should be handled. Since the balance developed in Eq. 4.15 applies to a single tracer step, if tracers are allowed to cross the interface without modification, then post-step concentration gradients near the interface will arise - i.e., on average, tracers moving into the high diffusivity medium will propagate less into the new medium than tracers moving into the low diffusivity medium. To remove post-step concentration gradients, tracers crossing an interface are first moved to the interface, their diffusivity is set to that of the new medium, and the following diffusive step is randomly sampled until the final position of the tracer lies within the new medium. An outline of the algorithm is given in Figure 4.2.
Despite the simple nature of the system considered (equilibrium diffusion in a composite medium), the modifications made to the random walk algorithm are applicable to much broader classes of problems. If the tracer step is kept small with respect to the particle diameter ($D_p$), then the effects of particle curvature may be neglected and the analytical solution for the 1D system holds, due to isotropy of the Gaussian distribution. Furthermore, the velocity field considered here will be continuous and nearly divergence free, due to nearly incompressible flow with no-slip boundary conditions imposed upon particle surfaces, and thus, requires no modification. Therefore, the given modifications may be extended to 3D, gas-solid systems involving flow.

4.4 Verification Simulations

To ensure that the new hybrid LBM-RWPT framework (implementation of Eq. 4.18 and Fig. 4.2) is correct, a variety of systems are simulated. Outputs from the new LBM-RWPT code are compared to analytical solutions, finite difference numerical solutions, empirical correlations, and previous DNS work. Note that simulation parameters for the LBM ($u$, $t$, $D_p$, $\rho$, $\eta$) and RWPT
method ($\alpha$) must be non-dimensionalized since the time step and grid spacing in LBM-RWPT are scaled to be unity [56]. To prevent ambiguity, quantities in physical space will be given alongside units while simulation inputs will be dimensionless.

4.4.1 Case 1: Effective Diffusivity of a Static Gas-Solids Mixture

The first case considered with the new code is conduction within a static gas-solids matrix. The matrix is unbounded and comprised of randomly located, non-overlapping, spheres within a fluid. A thermal impulse is applied to the matrix and the resulting conduction allows an effective diffusivity for the two-phase matrix to be quantified. The system in question is a natural starting point for verifying the new methodology and critically tests three key aspects. First, the simulations assess whether the phase biasing by tracers has been rectified. Namely, if tracers preferentially sample the lower diffusivity medium, then the effective diffusivity of the matrix will be significantly reduced from the true value. Second, the simulations are 3D and employ spherical particles within a cubic domain. Therefore, the assertion that the analytical solution may be extended to more complex geometries is evaluated. Third, the simulations are not at steady-state, and thus show whether the derived solution (Eq. 4.18) still holds in the transient state (based on definition of the equilibrium state). Furthermore, an analytical solution [57] as well as rigorous bounds [58] are known for the effective diffusivity of the matrix. The analytical solution of [57] is given by:

$$\alpha_{eff} = \alpha_f \left[ 1 - 3 \left( \frac{\alpha_s - \alpha_f}{\alpha_s + 2\alpha_f} \right) \varepsilon_s + \psi \varepsilon_s^2 \right]$$

(4.19)

$$\psi = 0.11, 0.208, 1.23, 3.90 \quad for \quad \frac{\alpha_s}{\alpha_f} = 0.5, 2.0, 5.0, 50.0$$

where $\alpha_{eff}$ is the effective diffusivity of the matrix, $\alpha_f$ is the diffusivity of the fluid, $\alpha_s$ is the diffusivity of the solids, $\varepsilon_s$ is the solids volume fraction, and $\psi$ is the coefficient of the second order solids volume fraction term; while the bounds determined numerically [58] are:
\[ \alpha_{\text{eff, LB}} = \left( \frac{1}{\alpha} - \frac{4\epsilon_g \epsilon_s \left( \frac{1}{\alpha_s} - \frac{1}{\alpha_f} \right)^2}{\frac{6}{\alpha_f} + (4\epsilon_g + 2\omega) \left( \frac{1}{\alpha_s} - \frac{1}{\alpha_f} \right)} \right)^{-1} \]  

(4.20)

\[ \alpha_{\text{eff, UB}} = \left( \langle \alpha \rangle - \frac{\epsilon_g \epsilon_s (\alpha_s - \alpha_f)^2}{3\alpha_f + (\epsilon_g + 2\omega) (\alpha_s - \alpha_f)} \right) \]

\[ \omega = 0.21068\epsilon_s - 0.04693\epsilon_s^2 + 0.00247\epsilon_s^3 \]

where \( \alpha_{\text{eff, LB}} \) is the lower bound for the effective diffusivity, \( \epsilon_g \) is the fluid volume fraction, \( \alpha_{\text{eff, UB}} \) is the upper bound for the effective diffusivity, \( \omega \) is a structure factor (determined by [58] via Monte Carlo simulation), and \( \langle X \rangle = \epsilon_g X_1 + \epsilon_s X_2 \) is the volume fraction weighted average. To determine the \( \alpha_{\text{eff}} \) within the new LBM-RWPT code, we employ the methods as outlined in [49, 51]; where \( \alpha_{\text{eff}} \) is given by the time rate of change of the mean dispersion of the tracers:

\[ \bar{M}_2 = \langle rr - \langle r^2 \rangle \rangle \]  

(4.21)

\[ \bar{\alpha}_{\text{eff}} = \lim_{t \to \infty} \frac{1}{2} \frac{d\bar{M}_2}{dt} \]

where \( \bar{M}_2 \) is the dispersion tensor and \( \langle \cdot \rangle \) refers to an average over all Brownian tracers. For the simulations here, the tracers are initialized uniformly in a plane located at the vertical centerline of the domain \( (y_{\text{min}} + y_{\text{max}})/2) \). Therefore, dispersion only occurs in the vertical \( y \)-direction and Eq. 4.21 may be simplified to

\[ \alpha_{\text{eff}} = \lim_{t \to \infty} \frac{1}{2} \frac{d}{dt} \left[ \langle r_y r_y - \langle r_y^2 \rangle \rangle \right]. \]  

(4.22)

Since the effective diffusivity will depend upon the matrix structure (particle locations), ten random particle configurations are generated for every diffusivity ratio \( (\alpha_s/\alpha_f) \). The number of particles within the matrix is held constant at 50 (\( \epsilon_s = 0.21 \)). A 95% confidence interval is utilized
to compare the output obtained from the new code to the closures proposed by [57, 58]. All domain walls are simulated with periodic boundary conditions and an overview of the simulation conditions is given in Table 4.1. As shown in Figures 4.3 - 4.6 for the various diffusivity ratios examined, outputs from the new code are observed to be in agreement with prior analytical predictions [57] and numerical bounds [58], whereas the original code [42, 43], which does not contain any modification for discontinuous diffusivity fields, under-predicts $\alpha_{eff}$ because tracers preferentially sample the lower diffusivity medium (phase biasing), resulting in an $\alpha_{eff}$ that is reduced from the true value. By contrast, the modifications developed here ensure that the tracers properly sample both phases. Note that the lower bound in [58] is essentially identical to the analytical solution obtained by [57]. This can be traced back to the homogenous particle distribution assumed by [57], whereas [58] obtains bounds upon $\alpha_{eff}$ which depend upon the arrangement of particles. Ultimately, no statistical difference is found between the $\alpha_{eff}$ obtained from the new code and that of [58].
Table 4.1: Simulation inputs for effective diffusivity simulations.

<table>
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<tr>
<th>Geometry and Operating Conditions</th>
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<tbody>
<tr>
<td><strong>LBM-RW Space</strong></td>
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<td>Number of Cells</td>
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<tr>
<td>$R_{p,LBM}$</td>
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<tr>
<td>$\varepsilon_s$</td>
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<td>$C_t$</td>
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<td>$\alpha_{f,RW}$</td>
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<td>Physical Space</td>
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<tr>
<td>$R_p$</td>
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<td>$\alpha_f$</td>
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Figure 4.3: (left) The effective diffusivity obtained for each matrix configuration and (right) the resulting confidence interval, for a diffusivity ratio of 0.5.

Figure 4.4: (left) The effective diffusivity obtained for each matrix configuration and (right) the resulting confidence interval, for a diffusivity ratio of 2.
Figure 4.5: (left) The effective diffusivity obtained for each matrix configuration and (right) the resulting confidence interval, for a diffusivity ratio of 5.

Figure 4.6: (left) The effective diffusivity obtained for each matrix configuration and (right) the resulting confidence interval, for a diffusivity ratio of 50.
4.4.2 Case 2 (Analytical Verification): Hot Sphere in Unbounded Diffusion

For the case of a hot sphere ($T_s$) suddenly immersed in an unbounded, static, cold fluid ($T_f$), the spherical heat balance only retains the temporal and radial components. If the sphere is kept at a constant temperature (Dirichlet), the analytical solution for the temperature profile and Nusselt number may be found via a similarity transform (i.e., combination of variables):

$$\theta(r, t) \equiv \frac{T(r, t) - T_f}{T_s - T_f} = \frac{R_p}{r} \left(1 - erf \left(\frac{r - R_p}{\sqrt{4\alpha f t}}\right)\right)$$  \hspace{1cm} (4.23)

$$Nu(t) \equiv \frac{hD_p}{k_f} = 2 + \frac{R_p}{\sqrt{\pi} \alpha f t}$$  \hspace{1cm} (4.24)

where $R_p$ is the radius of the sphere, $h$ is the heat transfer coefficient and $k_f$ is the thermal conductivity of the fluid. To make a comparison between the new code and the analytical Nusselt number (Eq. 4.24), a heat transfer coefficient ($h$) must be defined for the RWPT method. First, a temperature gradient ($T_s - T_f$) within the system is imposed by defining two types of tracers. Tracers labeled as type B correspond to $T_s (T_{hot})$ and A type tracers correspond to $T_f (T_{cold})$. The local temperature then becomes:

$$T(r, t) = T_s \frac{C_B(r, t)}{C_t} + T_f \frac{C_A(r, t)}{C_t}$$  \hspace{1cm} (4.25)

where $C_B$ is the concentration of B tracers, $C_A$ is the concentration of A tracers, and $C_t$ is the total tracer concentration. If the temperatures are chosen such that $T_f = 0$ and $T_s = 1$ then the B type tracers represent the temperature field solely ($T(r, t) = C_B(r, t)/C_t$). By definition, the heat transfer coefficient relates the heat flux ($q^-$) to the far field thermal temperatures ($q^- = h(T_s - T_f)$).

In the RWPT method, $q^-$ will be proportional to the net number of B type tracers crossing the particle interface per time. Therefore, if the net flux of B tracers across the surface of the sphere can be converted to thermal energy, then the heat transfer coefficient may be directly evaluated ($q^- = h(T_s - T_f) = h$). To accomplish this, the thermal energy corresponding to one B tracer...
within an LBM-RWPT cell (unit volume) is found via:

\[
E_t = V_{PS} (C_{v,f} \Delta t) = dx_{PS}^3 \left( C_{v,f} \frac{1}{C_t} \right)
\]

(4.26)

where \(E_t\) is the energy corresponding to \(C_B = 1\), \(V_{PS}\) is the volume of a LBM-RWPT cell in physical space, \(C_{v,f}\) is the volumetric heat capacity of the fluid (assumed equal to the solids, at this point), and \(dx_{PS}^3\) is the conversion factor between LBM-RWPT space and physical space. The heat flux and heat transfer coefficient then become:

\[
h = \frac{q}{\Delta T} = \left( \frac{\text{Net } \# \text{ B tracers crossing}}{A_p \Delta t} \right) \left( dx_{PS}^3 \left( C_{v,f} \frac{1}{C_t} \right) \right)
\]

(4.27)

where \(A_p\) is the area of the sphere, \(\Delta t\) is the number of LBM time steps over which the heat flux (net number of B tracers) is accumulated. Note that Eq. (4.27) is simply converting the flux of B tracers (left term in parenthesis) to thermal energy by way of the energy per tracer (middle term in parenthesis).

To satisfy the required initial condition and boundary condition for the unbounded diffusion case, special attention must be given to how the tracer type is set. All tracers are initialized uniformly over the entire system domain but those lying within the sphere are set to type B while those in the fluid are set to type A. Physically, this initialization is analogous to a uniform temperature of \(T_s\) within the sphere and a uniform temperature of \(T_f\) within the fluid (Eq. 4.25). To maintain the sphere at \(T_s\) (Dirichlet), all tracers entering the sphere are set to type B. Furthermore, the domain walls are again treated as periodic and an outline of the simulation conditions is given in Table 4.2. The Nusselt numbers obtained from simulations are observed to be in strong agreement with the analytical solution (Eq. 4.23) over a variety of diffusivity ratios; see Fig. 4.7. The local, dimensionless concentration of all tracers \((\theta_t(\mathbf{r}) = (C_B(\mathbf{r}) + C_A(\mathbf{r}))/C_t)\) and B tracers \((\theta_B(\mathbf{r}) = (T(\mathbf{r}) - T_f)/(T_s - T_f) = C_B(\mathbf{r})/C_t)\) is illustrated in Figure 4.8. A cubic grid \((4 \times 2 \times 4)\) is employed to decompose the domain and calculate the local concentrations. \(\theta_t\) is observed to be homogenous over the entire domain and equal to one (Fig. 4.8). Since the system is initialized at
equilibrium, with respect to all the tracers, this result supports the fact that the modifications to the RWPT algorithm properly maintain equilibrium (Eq. 4.15 is satisfied). By contrast, $\theta_B(r)$ not only varies spatially but decreases as the radial position from the particle surface is increased (Fig. 4.8), which agrees with the analytical solution (Eq. 4.23).

Table 4.2: Simulation inputs for unbounded diffusion simulations.

<table>
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<tr>
<th>Geometry and Operating Conditions</th>
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<tbody>
<tr>
<td><strong>LBM Space</strong></td>
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<tr>
<th><strong>Physical Space</strong></th>
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<tbody>
<tr>
<td>$R_p$</td>
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<tr>
<td>$\alpha_f$</td>
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<tr>
<td>$k_f$</td>
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<tr>
<td>$C_v,f$</td>
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</tbody>
</table>
Figure 4.7: The Nu number achieved via simulation compared to the analytical solution, for a diffusivity ratio of 0.5, 1, 5.

Figure 4.8: (left) The dimensionless total tracer concentration ($\theta_t$) and (right) the dimensionless B tracer concentration ($\theta_b$) (temperature field) at a time of $1 \times 10^{-3}[s]$ and $\alpha_s/\alpha_f = 5$, where the dashed line denotes the outline of the sphere.
4.4.3 Case 3 (Numerical Verification): Cooling Sphere in Unbounded Diffusion

Under the conditions given in Section 3.2 (Hot Sphere in Unbounded Diffusion), the coupling of heat transfer between the sphere and the fluid is only one-way coupled. Namely, as the sphere transfers heat to the fluid it does not in turn cool but remains at a constant temperature. Here, we allow the sphere to cool, and thus, develop intra-particle temperature gradients in the radial direction. Due to the added complexity of coupling the two phases, an analytical solution cannot be found for the temperature profile. Instead, the simulation outputs are compared to results from a finite difference (FD) code. The FD algorithm discretizes the spherical heat balance on a staggered grid [59] over the span of \([0, 3R_p]\) with a symmetry boundary condition at \(r = 0\) [60] and an adiabatic boundary condition at \(r = 3R_p\) [61]:

\[
\frac{\partial T}{\partial t} = \begin{cases} 
\frac{6k_1/2\Delta t}{C_v,0\Delta r^2}(T_1 - T_0) & \text{for } i = 0 \\
\frac{2k_{N-1/2}\Delta t}{C_v,N\Delta r^2}(T_{N-1} - T_N) & \text{for } i = N \\
\frac{1}{C_v,i}\left[\frac{r_{i+1/2}^2k_{i+1/2}}{\Delta r^2}T_{i+1} - \frac{r_{i+1/2}^2k_{i+1/2} + r_{i-1/2}^2k_{i-1/2}}{\Delta r^2}T_i + \frac{r_{i-1/2}^2k_{i-1/2}}{\Delta r^2}T_{i-1}\right] & \text{else}
\end{cases}
\]

(4.28)

where \(i\) denotes the node index and \(N\) is the total number of nodes \((10^3)\). The temporal derivative in Eq. (4.28) is approximated by an implicit Euler scheme and the resulting matrix equation is solved by the generalized minimal residual method (GMRES).

Since both phases are coupled in the current case, the temporal change in particle temperature is given by the net flux of thermal energy across the interface - i.e., the application of Eq. (4.7) to particle and fluid. The amount of thermal energy gained by the fluid must be equal to the thermal energy lost by the particle. If an energy balance is performed at the fluid-particle interface, it can be seen that this criterion is only met if the volumetric heat capacities of both phases are equal \((C_{v,s} = C_{v,f})\):

\[
\Delta E = (N_{B,f\to s} - N_{B,s\to f}) \left(\frac{C_{v,s}}{C_t}\right) + (N_{B,s\to f} - N_{B,f\to s}) \left(\frac{C_{v,f}}{C_t}\right) = \Delta N_{B,s} \left(\frac{C_{v,f}}{C_t}\right) (1 - \gamma) \tag{4.29}
\]
\[ \Delta N_{B,s} = (N_{B,s \rightarrow f} - N_{B,f \rightarrow s}), \quad \gamma = \frac{C_{v,s}}{C_{v,f}} \]

where \( \Delta E \) is the change in energy between the two phases, \( N_{B,f \rightarrow s} \) is the number of B tracers crossing from fluid to solid, \( N_{B,s \rightarrow f} \) is the number of B tracers crossing from solid to fluid, \( \frac{C_{v,s}}{C_{l}} \) is the energy per tracer in the solid phase, \( \frac{C_{v,f}}{C_{l}} \) is the energy per tracer in the fluid phase, \( \Delta N_{B,s} \) is the net change in B tracers in the solid phase, and \( \gamma \) is the ratio of volumetric heat capacities. A net energy change when \( C_{v,s} \neq C_{v,f} \) can be attributed to the fact that a tracer represents a different amount of energy in the solid phase than the fluid phase. Thus, if tracer types are merely exchanged across the interface then the continuum equation (4.7) will not be satisfied, unless \( C_{v,s} = C_{v,f} \) - i.e., the temporal change in temperature (post-step tracer concentration) will be improperly characterized due to tracers representing different amounts of energy in each phase. To address the challenge of unequal volumetric heat capacities, A type tracers entering the high volumetric heat capacity medium are converted to B type. Specifically, the number of tracers which should be converted is found by:

\[ \Delta E = (N_{B,\text{Conv}} - \Delta N_{B,s}) \left( \gamma \frac{C_{v,f}}{C_{l}} \right) + \Delta N_{B,s} \left( \frac{C_{v,f}}{C_{l}} \right) = 0 \quad \text{for } \gamma > 1 \quad (4.30) \]

\[ \therefore N_{B,\text{Conv}} = \frac{\gamma - 1}{\gamma} \Delta N_{B,s} \]

\[ \Delta E = (-\Delta N_{B,s}) \left( \frac{C_{v,s}}{C_{l}} \right) + (\Delta N_{B,s} - N_{B,\text{Conv}}) \left( \frac{1}{\gamma} \frac{C_{v,s}}{C_{l}} \right) = 0 \quad \text{for } \gamma < 1 \quad (4.31) \]

\[ \therefore N_{B,\text{Conv}} = (1 - \gamma) \Delta N_{B,s} \]

where \( N_{B,\text{Conv}} \) is the number of A tracers entering the high heat capacity medium that should be converted to B tracers. Since \( N_{B,\text{Conv}} \) is a function of the net number of B tracers crossing the particle interface (\( \sim q^{\gamma} \)), it is calculated at the end of the tracer loop and the conversion of the
Simulation inputs for each heat capacity ratio ($\gamma = 0.1, 1, 10$) match the $\alpha_s/\alpha_f = 0.5, 5$ cases in Table 4.2 and the domain boundary conditions are identical to those in Section 3.2. The dimensionless temperature profiles ($\theta_B(\hat{r})$, $\hat{r} = r/R_p$) obtained from simulations are found to be in agreement with those obtained via the FD approximation; see Figures 4.9 - 4.11 for different values of heat capacity and thermal diffusivity ratios. The profiles are extracted from the code by decomposing the domain into 50 concentric spherical shells and calculating $\theta_B$ on each shell. While the shells naturally address the radial dependence of the problem, the shell volume becomes small as $\hat{r} \to 0$ and leads to noise in $\theta_B$ near the center of the particle. For some of the cases under consideration here, the particle conductivity ($k_s$) is small with respect to the fluid conductivity ($k_f$) ($k_s/k_f < 1$). Physically, this condition results in thermal energy being redistributed within the sphere at a slower rate than the fluid. For cases in which $k_s/k_f = \gamma(\alpha_s/\alpha_f) < 1$, both the RWPT code and the FD code show substantial temperature gradients near the surface of the sphere; see Fig. 4.9 and 4.10 (left). A common assumption made within DNS or the discrete element method (DEM) is that spheres are isothermal - i.e., the Biot number ($Bi = hD_p/k_s$) is small, and thus, intra-particle thermal gradients are negligible. Recent work has highlighted the challenges associated with resolving intra-particle temperature gradients [62, 63]. The RWPT method developed here shows promise for being able to capture the heat transfer occurring in systems with large Biot numbers and does not suffer the computational overhead associated with carrying a highly resolved numerical grid for each particle.
Figure 4.9: The dimensionless B tracer concentration ($\theta_b$) as a function of dimensionless radius ($\hat{r}$) for (left) $\gamma = 0.1$, $\alpha_s/\alpha_f = 0.5$ and (right) $\gamma = 0.1$, $\alpha_s/\alpha_f = 5$.

Figure 4.10: The dimensionless B tracer concentration ($\theta_b$) as a function of dimensionless radius ($\hat{r}$) for (left) $\gamma = 1$, $\alpha_s/\alpha_f = 0.5$ and (right) $\gamma = 1$, $\alpha_s/\alpha_f = 5$. 
Figure 4.11: The dimensionless B tracer concentration ($\Theta_b$) as a function of dimensionless radius ($\hat{r}$) for (left) $\gamma = 10$, $\alpha_s/\alpha_f = 0.5$ and (right) $\gamma = 10$, $\alpha_s/\alpha_f = 5$.

4.4.4 Case 4 (Validation): Uniform Flow Past a Hot Sphere

The final case considered with the new LBM-RWPT code is that of unbounded flow of a cold fluid past a stationary, hot sphere. Here, the ability of the new framework to characterize non-isothermal flows is assessed. Comparisons are made between the new code and experiments [64, 65], as well as earlier numerical studies [27, 66]. Thus, the ability of the new hybrid code to accurately capture flow and transport (validation) is completed, not just the recovery of a known accurate solution (verification) [67]. Previous works [21, 38, 52] show strong agreement between numerical predictions and state-of-the-art correlations for the Nusselt number. We compare the Nusselt number obtained via the LBM-RWPT code, at intermediate Reynolds numbers ($Re = 10, 20, 30, 40, 50, 100$) and a Prandtl number ($Pr$) of 0.7, to the correlations given by Ranz and Marshall [64], Whitaker [65], Feng and Michaelides [27], and Richter and Nikrityuk [66], respectively:
\[ Nu = 2.0 + 0.6Re^{1/2}Pr^{1/3} \]  \hspace{1cm} (4.32)

for \( 10 < Re < 10^4,\ Pr > 0.7 \)

\[ Nu = 2.0 + \left( 0.4Re^{1/2} + 0.06Re^{2/3} \right)Pr^{0.4} \]  \hspace{1cm} (4.33)

for \( 3.5 < Re < 7.6 \times 10^4,\ 0.7 < Pr < 380 \)

\[ Nu = 0.992 + Pe^{1/3} + 0.1Re^{1/3}Pe^{1/3} \]  \hspace{1cm} (4.34)

for \( 0.1 < Re < 4 \times 10^3,\ 0.2 < Pe < 2 \times 10^3 \)

\[ Nu = 1.76 + 0.55Re^{1/2}Pr^{1/3} + 0.014Re^{2/3}Pr^{1/3} \]  \hspace{1cm} (4.35)

for \( 10 < Re < 250,\ Pr > 0.7 \)

where \( Pe = RePr \) is the Peclet number. The hydrodynamic and thermal boundary conditions are as follows:

1. Uniform axial inflow \( \mathbf{u} = [0 \ U_{0,y} \ 0] \) and temperature \( T = T_f \) at the inlet plane \( (y = y_{min}) \);
2. Zero gradient in the stream wise direction \( \left( \frac{\partial \mathbf{u}}{\partial y} = 0, \ \frac{\partial T}{\partial y} = 0 \right) \) at the outlet plane \( (y = y_{max}) \)
3. Periodic in the x and z direction; and
4. Constant temperature sphere \( T = T_s \) with no slip \( (\mathbf{u} = 0) \) at the surface

Enforcement of the axial inflow and the no slip boundary conditions are accomplished by the modified bounce-back method of Ladd [53] while the outflow is achieved by extrapolation of the
incoming distribution functions \cite{38, 68, 69}. The particle is maintained at a constant temperature in the same manner as discussed in Section 3.2. Thermal boundary conditions at the inflow/outflow boundary are achieved by a two-step approach. If a tracer crosses the outflow plane, it is then randomly reseeded along the inflow plane and its type is set to A. Whereas, if a tracer crosses the inflow plane, it is specularly reflected and its type is set to A. The grid resolution employed here ($D_{p, LBM} = 20$) has been shown by previous work \cite{21, 38, 52} to achieve the required accuracy over the aforementioned Reynolds numbers. Furthermore, to minimize boundary effects and achieve an unbounded flow, the domain sizes of \cite{52, 70} are utilized ($8D_p \times 16D_p \times 8D_p$). The thermal diffusivity ratio is held constant for these simulations ($\alpha_s/\alpha_f = 5$) and the fluid thermal diffusivity is set to $\alpha_f = 2.23 \times 10^{-5}\frac{[m^2]}{[s]}$.

Nusselt numbers found by the new LBM-RWPT code are observed to agree with the correlations of \cite{27, 64–66}; see Figure 4.12. Verification studies by \cite{21, 38, 52} show similar results. Furthermore, the $\theta_l$ is again observed to be nearly homogenous (Figure 4.13 (left)) while the $\theta_B$ displays a thin boundary layer of hot fluid around the sphere with a wake of warm fluid following behind it (Figure 4.13 (right)) - i.e., the expected qualitative behavior.
Figure 4.12: The Nu number as a function of sphere Reynolds number achieved via LBM-RWPT simulations and state-of-the-art correlations.

Figure 4.13: (left) The dimensionless total tracer concentration ($\theta_t$) and (right) the dimensionless B tracer concentration ($\theta_b$) (temperature field) at steady-state and $Re = 40$, where the dashed line denotes the outline of the sphere.
4.4.5 Concluding Remarks

A technique for simulating heat (or mass) transfer in multiphase systems via a hybrid lattice Boltzmann method (LBM) - random walk particle tracking (RWPT) method is presented here. Analytical methods were utilized to modify the RWPT algorithm for use in systems with discontinuous diffusivity fields, which past RWPT works were unable to account for. An interfacial tracer balance was combined with the definition of equilibrium to determine how the stochastic movement of tracers should be altered. By expanding the displacement tensor for the higher diffusivity medium and only allowing a subset of the tracers within the higher diffusivity medium to undergo stochastic movement, the tracer balance across an interface can be satisfied at equilibrium. Furthermore, a means for quantifying the heat transfer coefficient in the RWPT framework, as well as a technique for handling differing volumetric heat capacities, was developed. The energy per tracer is employed to convert the flux of tracers to a heat transfer coefficient as well as develop an energy balance at the interface of the two mediums. The algorithm is verified against four test cases to ensure that it recovers the correct macroscopic transport phenomena. Outputs from the new LBM-RWPT code are observed to be in agreement with past analytical/numerical solutions as well as empirical correlations and previous works.

The hybrid method developed in the present work offers a variety of advantages for simulating systems with scalar transport. Namely, the RWPT is a meshless method that does not suffer from numerical dispersion and is straightforward to implement/parallelize, unlike classic finite difference and finite element methods. Furthermore, the present work demonstrates the potential of RWPT to capture intra-particle temperature gradients, and thus, may be a valuable alternative for the simulation of heat transfer in high Biot number systems, since it does not suffer the computational overhead associated with a highly-resolved grid for each particle. While not considered in the present work, the particles may also translate in space. However, further development of the method is required to handle such cases. Specifically, the tracers may change phase due to the discrete particle motion over the tracer field. The creation and destruction of solid or fluid type
tracers must be handled in a rigorous fashion to ensure the proper physics are retained. Means for addressing medium motion will be the subject of future work.

At this point, the DNS code has been modified for multiphase systems and verified for a variety of case studies. While it may be tempting to now assess the validity of indirect conduction theory for wall-bounded gas-solids flows, some small challenges still remain. Namely, none of the case studies considered here involved the presence of a wall. While this subtlety may seem trivial, it will be shown in Chapter 5 that the presence of a no-slip wall causes significant challenges to the random walk algorithm at the outflow plane. Introduction of the no-slip wall results in fluid velocities at the outflow plane than range from zero to the free-stream velocity. Therefore, the outflow plane is characterized by regions that continuously range from diffusion dominated (near-wall) to advection dominated (free-stream). Treatments for a completely diffusion dominated (impenetrable method used here) and advection dominated (open method used here) boundary have been well established but no means exist for the intermediate case. In Chapter 5 a semi-reflecting barrier will be derived and shown to be a general method for enforcing an outflow boundary condition on the random walk framework.
4.5 Chapter 4 Bibliography


Chapter 5

A Fully-Developed Boundary Condition for the Random Walk Particle Tracking Method

5.1 Abstract

Random walk particle tracking (RWPT) is an effective and flexible approach to resolve scalar transport in direct numerical simulations (DNS) of single and multi-phase flows. It is often part of a hybrid scheme where the flow field is recovered by a separate hydrodynamic solver and the scalar field is resolved by RWPT. Since RWPT method tracks the displacement of passive Brownian tracers, rather than discretizing the advection-diffusion equation, development of boundary conditions for RWPT is not trivial. Namely, rules imposed upon a single tracer at the boundary must, after averaging, recover the desired continuum scale boundary condition. Here we develop means for imposing a fully-developed outflow boundary condition for the RWPT method. The technique developed here utilizes a semi-reflecting barrier at the outflow boundary. Tracers that reach the boundary plane are either reflected back into the domain or allowed to vacate the domain. We show that the semi-reflecting barrier developed here converges to the classic reflective boundary and open boundary in the asymptotic limit of low and high Peclet number, respectively. The new outflow boundary condition is verified against boundary layer (BL) theory for flow past a hot plate. The temperature field extracted at the outflow boundary is observed to be in agreement with BL solutions.

5.2 Introduction

The random walk particle tracking (RWPT) method has been shown to be an effective method for solving the advection-diffusion equation. Commonly, RWPT is coupled to a hydrodynamic solver to resolve scalar transport (concentration or temperature). Since RWPT relies upon tracking passive tracer particles, it does not suffer from numerical dispersion in advection-dominated flows \[1\], is readily extendable to complex geometries \[2, 3\], and can handle non-Fickian transport \[4\]. The advantages of RWPT have led to its application to a diverse group of systems \[5–8\]. Despite the varied use of RWPT, means for rigorously imposing a fully developed outflow boundary condition within the algorithm have not been established.

We propose a method for enforcing a fully-developed outflow boundary in hybrid RWPT methods where the velocity field (\(\mathbf{u}\)) is recovered via a hydrodynamic solver and the scalar field (concentration or temperature) is obtained by RWPT. A fully-developed boundary condition at the exit is characterized by a zero gradient in both the velocity (\(\mathbf{u}\)) and scalar field (\(T\)) in the direction of the outward normal of the boundary plane (\(\mathbf{n}\)) - i.e., \(\frac{\partial \mathbf{u}}{\partial n} = 0\) and \(\frac{\partial T}{\partial n} = 0\). The present work establishes a method for imposing \(\frac{\partial T}{\partial n} = 0\) on the RWPT method subject to the constraint that \(\frac{\partial \mathbf{u}}{\partial n} = \mathbf{0}\) is already achieved by the hydrodynamic solver. The technique developed here employs a semi-reflecting barrier at the outflow boundary. Tracer particles that reach the boundary plane are either reflected back into the domain or allowed to vacate the domain. We created a fictitious mirror image of the near-boundary region and allowed the tracers to undergo a single displacement step. The mirror image inherently satisfies the zero gradient criterion and allows the probability of a tracer being reflected to be found analytically. We show that the classic reflective boundary \[6, 9\] and open boundary \[10\] are not general methods for achieving fully developed flow at the exit, but are instead the asymptotic behavior of the semi-reflecting barrier developed here and are valid in the low and high Peclet number limits, respectively. The new outflow boundary condition was implemented within a hybrid lattice Boltzmann - random walk (LBM-RWPT) algorithm \[10\] and utilized to simulate uniform flow past a hot plate. The temperature field at the outflow boundary
was observed to be in reasonable agreement with boundary layer theory over a wide range of Prandtl numbers.

5.3 Numerical Techniques

5.3.1 Lattice Boltzmann Method (LBM)

The lattice Boltzmann method (LBM) is utilized in this work to solve the Navier-Stokes (NS) equations. Specifically, the algorithm employed here matches that in [11–13]. Instead of a discretization of the NS equations themselves, LBM is based on a discretization of the continuous Boltzmann equation. Therefore, LBM simulates the evolution of molecular velocity distributions (population densities) as opposed to the hydrodynamic variables. Updates to the discrete velocity distributions are carried out through repeated streaming and collision:

\[ n_i(r + c_i \Delta t, \Delta t) \equiv n_i^*(r, t) = n_i(r, t) + \Omega_i(n(r, t)) \quad (5.1) \]

where \( n_i \) is the discrete velocity distribution (population density of molecules at position \( r \) with a velocity \( c_i \)), \( \Delta t \) is the LBM time step (scaled to be unity), \( \Omega_i \) is the collision operator, and \( n_i^* \) is the post-collision distribution function. A linearized collision operator was used in the present work and and matches that in [13]. The hydrodynamic quantities correspond to moments of the discrete distribution functions:

\[ \rho = \sum_i n_i \quad j \equiv \rho \mathbf{u} = \sum_i n_i \mathbf{c}_i \quad \tilde{\Pi} = \sum_i n_i \mathbf{c}_i \mathbf{c}_i \quad (5.2) \]

where \( \rho \) is the density, \( j \) is the momentum, and \( \tilde{\Pi} \) is the fluid stress tensor. Via a Taylor expansion of the finite difference approximation in Eq. 5.1 and a Chapman-Enskog expansion, it can be shown that LBM recovers the Navier-Stokes equations with the following closures for the shear (\( \eta \)) and bulk (\( \eta_b \)) viscosities [13]:

\[ \eta = -\rho c_s^2 \left[ \frac{1}{\lambda} + \frac{1}{2} \right] \quad \eta_b = -\frac{2\rho c_s^2}{3} \left[ \frac{1}{\lambda_b} + \frac{1}{2} \right] \quad (5.3) \]
where \( c_s^2 = \frac{1}{3} \) is the square of the speed of sound, \( \lambda \) and \( \lambda_b \) are eigenvalues of the collision matrix. \( \lambda \) corresponds to the relaxation of the off diagonal portion of the non-equilibrium stress tensor while \( \lambda_b \) corresponds to the relaxation of the diagonal portion of the non-equilibrium stress tensor.

**5.3.2 Random Walk Particle Tracking (RWPT)**

The RWPT method is employed here to resolve the scalar transport of thermal energy, as governed by the advection-diffusion equation:

\[
\frac{\partial T}{\partial t} + u \cdot \nabla (T) = \alpha \Delta (T) \tag{5.4}
\]

where \( T \) is the thermal temperature and \( \alpha \) is the thermal diffusivity. If the positions of many tracer particles are updated according to a Langevin equation, the resulting distribution of tracer particles can be shown to recover Eq. 5.4. Thus, rather than discretizing Eq. 5.4, RWPT monitors the positions of many Brownian tracers as they undergo movement that depends upon the local velocity field and random fluctuations. Here we utilize the Euler-Maruyama integration scheme for stochastic differential equations (SDEs) to evolve the position of each tracer:

\[
\mathbf{r}_i(t + \Delta t) = \mathbf{r}_i(t) + u(\mathbf{r}_i, t)\Delta t + \mathbf{\xi}(t)\sqrt{2\alpha\Delta t} \tag{5.5}
\]

where \( \mathbf{r}_i \) is the position of tracer \( i \), \( u \) is the velocity at the tracer position before the step (found via trilinear interpolation of the LBM velocity field in this work), and \( \mathbf{\xi} \) is a random vector whose entries are sampled from a Gaussian distribution with zero mean and unit variance. The thermal temperature then becomes proportional to the tracer concentration in RWPT. In this study, we mapped two temperatures, \( T_1 \) and \( T_0 \) \((T_1 > T_0)\), to concentrations of two tracer types. Tracers of type ’0’ are eliminated at the solid wall. Every elimination of a tracer of type ’0’ on the wall creates a tracer of type ’1’. The solid wall therefore can be thought of a sink for tracers of type ’0’ and a source for tracers of type ’1’. At the entrance, tracers of type ’1’ are eliminated and tracers
of type '0' are created. The temperature is defined as

\[ T(r, t) = T_1 \frac{C_1(r, t)}{C_t} + T_0 \frac{C_0(r, t)}{C_t} \]  

where \( C_1 \) is the concentration of type 1 tracers, \( C_0 \) is the concentration of type 0 tracers, \( C_t \) is the total tracer concentration in the domain which is a constant. This setup ensures that a constant temperature difference \( (\Delta T = T_1 - T_0) \) is maintained between the entrance and the solid wall. The dimensionless temperature \( \theta \) is then

\[ \theta(r, t) \equiv \frac{T(r, t) - T_0}{T_1 - T_0} = \frac{C_1(r, t)}{C_t} \]  

5.4 Boundary Condition Development

The reflective barrier is commonly employed to enforce a zero-flux condition at a (solid or symmetry) boundary. However, an outflow boundary will in general have a nonzero velocity in the direction normal to the wall \( (\mathbf{u} \cdot \mathbf{n} \neq 0) \). Since the displacement of tracers contains a deterministic portion \( (\mathbf{u}(r_i, t) \Delta t) \) in Eq. 5.5, the average displacement of tracers will be nonzero and in the direction of the local velocity field. Thus, if \( \mathbf{u} \cdot \mathbf{n} > 0 \) at the boundary, then tracers near the boundary will have an average displacement towards the boundary. Under these conditions, it can easily be seen that a reflective barrier (impenetrable) would lead to an accumulation of tracers in the near boundary region. To account for the effects of the hydrodynamic outflow boundary \( (\frac{\partial \mathbf{u}}{\partial n} = \mathbf{0}) \), a fictitious mirror image of the tracer distribution may be considered; see Figure 5.1. Since the tracer concentration in the near boundary region and the mirror image are the same, the temperatures associated with both sub volumes are the same and the zero-gradient condition \( (\frac{\partial T}{\partial n} = \mathbf{0}) \) is inherently satisfied.

If the tracers are allowed to undergo a displacement step, then there are four possible outcomes due to the random portion of the displacement in Eq. 5.5: (i) both real and fictitious tracers reach the boundary, (ii) only the real tracer reaches the boundary, (iii) only the fictitious tracer reaches the
boundary, or (iv) neither tracer reaches the boundary. The probability that a real tracer reaches the boundary is related to its separation distance from the boundary plane. Considering a generic plane given by

$$\mathbf{n} \cdot (\mathbf{x} - \mathbf{a}) = 0,$$

(5.8)

where $\mathbf{x} = [x \ y \ z]$ is the vector variable, $\mathbf{n}$ is again the unit normal vector pointing out of the domain, and $\mathbf{a}$ is a point contained within the outflow plane, the criterion for a tracer to reach the outflow plane becomes

$$\mathbf{n} \cdot (\mathbf{u}(\mathbf{r}_i, t) \Delta t + \xi \sqrt{2\alpha \Delta t}) \geq \mathbf{n} \cdot (\mathbf{a} - \mathbf{r}_i)$$

(5.9)

Considering a boundary aligned with the YZ plane, Eq. (5.9) is simplified to a single dimension and only the x-direction need be considered:

$$u_x(\mathbf{r}_i, t) \Delta t + \xi_x \sqrt{2\alpha \Delta t} \geq \delta_x$$

(5.10)
where \( \delta_x = a_x - r_{i,x}(t) \) is the separation distance between tracer \( i \) and the outflow plane. The probability of reaching the plane then becomes the probability of sampling a \( \xi_x \) such that Eq. 5.10 is satisfied:

\[
P(\delta_x^-) \equiv \int_{\delta_x^-}^{\infty} \frac{1}{\sqrt{2\pi}} e\left(-\frac{x^2}{2}\right) \, dx = \frac{1}{2} \text{erfc}\left(\frac{\delta_x^- - u_x(r_i)\Delta t}{2\sqrt{\alpha \Delta t}}\right)
\] (5.11)

where \( P(\delta_x^-) \) is the probability of a real tracer with separation distance \( \delta_x \) reaching the outflow plane. For mirror image tracers, the analogous probability is given by

\[
P(\delta_x^+) \equiv \int_{\delta_x^+}^{\infty} \frac{1}{\sqrt{2\pi}} e\left(-\frac{x^2}{2}\right) \, dx = \frac{1}{2} \text{erfc}\left(\frac{\delta_x^+ + u_x(r_i)\Delta t}{2\sqrt{\alpha \Delta t}}\right).
\] (5.12)

Since the stochastic steps sampled by two tracers are not correlated, the probability of the four outcomes are given by

i. \( P(\delta_x^-)P(\delta_x^+) \)

ii. \( P(\delta_x^-)(1 - P(\delta_x^+)) \)

iii. \( (1 - P(\delta_x^-))P(\delta_x^+) \)

iv. \( (1 - P(\delta_x^-))(1 - P(\delta_x^+)) \)

In outcomes (i) and (iii), a new tracer must be introduced into the near boundary region. Therefore, the probability of adding a new tracer becomes

\[
P(\delta_x^-)P(\delta_x^+) + (1 - P(\delta_x^-))P(\delta_x^+) = P(\delta_x^+)
\] (5.13)

Rather than dynamically introducing tracers at the outflow boundary according to Eq. 5.13, a subset of the tracers that reach the interface from the near boundary region may be specularly reflected. Therefore, the probability of a tracer being specularly reflected (Eq. 5.13), given that the tracer reached the interface (\( P(\delta_x^-) \)) is given by

\[
P^* \equiv \frac{P(\delta_x^+)}{P(\delta_x^-)} = \frac{\text{erfc}\left(\frac{\delta_x^+ + u_x(r_i)\Delta t}{2\sqrt{\alpha \Delta t}}\right)}{\text{erfc}\left(\frac{\delta_x^- - u_x(r_i)\Delta t}{2\sqrt{\alpha \Delta t}}\right)}
\] (5.14)
Implementation of the outflow boundary condition then becomes:

1. Test if tracer will cross the outflow boundary plane

2. If tracer will cross, calculate the separation distance ($\delta_x$) and the probability of being specularly reflected $P^*$ (Eq. 5.14).

3. Sample a random number from a uniform distribution on $[0, 1]$ ($\mathcal{U}(0,1)$). If the number is less than $P^*$, the tracer is specularly reflected. Else, the tracer is allowed to vacate the domain.

From Eq. 5.14 it can readily be seen that the probability of reaching the outflow plane will inherently depend upon the Peclet number ($Pe$):

$$P(\delta_x^{+-}) = \frac{1}{2} erfc \left( \frac{\delta_x}{2\sqrt{\alpha \Delta t}} \pm Pe(r_i) \frac{\sqrt{2}}{4} \right)$$

(5.15)

$$Pe \equiv \frac{L(u \cdot n)}{\alpha} = \frac{\sqrt{2 \alpha \Delta t u_x}}{\alpha}$$

(5.16)

where $P(\delta_x^{+-})$ is the probability of a real ($-$) or mirror image ($+$) tracer reaching the outflow plane and the sign within the complementary error function ($\pm$) is given by the sign of the superscript, $L = \sqrt{2 \alpha \Delta t}$ is the characteristic length scale, and $u \cdot n$ is the velocity in the normal direction to the outflow plane. Note that the second equality in Eq. 5.16 holds for the YZ plane considered in the present derivation and a characteristic length scale for the advection-diffusion equation. Expanding the probability of reaching the interface (Eq. 5.15) about $\delta_x = 0$ allows the asymptotic behavior of the outflow boundary (Eq. 5.14) in the high and low $Pe$ number to be seen. Namely, as the Peclet number becomes large (advection dominated) $P^*$ tends to zero and the outflow condition is achieved via an open boundary where all tracers that reach the boundary will vacate the domain. By contrast, as the Peclet number becomes small (diffusion dominated) $P^*$ tends to unity and the outflow condition is achieved via an impenetrable boundary where all tracers that reach the plane
will be specularly reflected into the domain i.e., the classic method for achieving an adiabatic boundary \( \frac{dT}{dn} = 0 \).

\[
P(\delta^+) \approx \frac{1}{2} \text{erfc} \left( Pe(r_i) \frac{\sqrt{2}}{4} \right) + O(\delta_x)
\]

\[
P(\delta^-) \approx 1 - \frac{1}{2} \text{erfc} \left( Pe(r_i) \frac{\sqrt{2}}{4} \right) + O(\delta_x)
\]

\[
\lim_{Pe \to \infty} P^* = 0
\]

\[
\lim_{Pe \to 0} P^* = 0
\]
5.5 Systems Simulated

To verify the outflow boundary condition given by Eq. 15, uniform flow past a hot plate is considered; see Figure 5.2.

![Figure 5.2: An illustration of the geometry and boundary conditions for flow past a hot plate.](image)

At steady state and large Reynolds numbers \((Re = \frac{U_{\infty}}{\nu}) \ (Re \geq 10^3)\), boundary layer (BL) theory makes use of the simplified Prandtl equations (rather than the Navier-Stokes equations) \([16, 18]\):

\[
\begin{align*}
\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} &= 0, \\
 u_x \frac{\partial u_x}{\partial x} + u_x \frac{\partial u_x}{\partial y} &= \nu \frac{\partial^2 u_x}{\partial y^2}.
\end{align*}
\]

(5.21)  
(5.22)

where \(u_x\) is the stream-wise velocity component, \(u_y\) is the span-wise velocity component, and \(\nu\) is the kinematic viscosity. By introducing the 2D stream function \((\mathbf{u} = \nabla \times (\psi \mathbf{e}_z))\), the continuity equation (Eq. 5.21) may be eliminated at the expense of increasing the order of the momentum
equation (Eq. 5.22)

\[ \frac{\partial \psi}{\partial y} \frac{\partial^2 \psi}{\partial x \partial y} - \frac{\partial \psi}{\partial x} \frac{\partial^2 \psi}{\partial y^2} = -\nu \frac{\partial^3 \psi}{\partial y^3} \]  

(5.23)

Introduction of the similarity variables \( \eta = y \sqrt{\frac{U_\infty}{2\nu x}} \) and \( \psi = f(\eta) \sqrt{2U_\infty \nu x} \) allows the third-order PDE given in Eq. 5.23 to be reduced to the following ordinary differential

\[ f''' + f f'' = 0. \]  

(5.24)

Tabulated data of the numerical solution to Eq. 5.24 may be found in many classic texts [16, 18]. To directly compare with BL theory, a simple and compact function which well approximates the hydrodynamic field (solution to Eq. 5.24) is desirable. Here we will employ an error function fit to the data given in [17]

\[ u_x(x, y) \approx U_\infty \text{erf} \left( 0.4542y \sqrt{\frac{U_\infty}{2\nu x}} \right) \]  

(5.25)

where \( U_\infty \) is the free-stream velocity in the stream-wise direction. The velocity fitting function (Eq. 5.25) is observed to be in reasonable agreement with the tabulated data of [17]; see Figure 5.3.

The thermal transport equation simplifies to the familiar steady-state advection-diffusion equation

\[ u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} = \alpha \frac{\partial^2 T}{\partial y^2}. \]  

(5.26)

By nondimensionalizing the thermal temperature and utilizing the same similarity variable (\( \eta \)) as above (\( \theta(\eta) = (T - T_\infty) / (T_w - T_\infty) \)), the advection-diffusion equation (Eq. 5.26) may be simplified to an ordinary differential

\[ \theta'' + Pr f \theta' = 0 \]  

(5.27)

where \( Pr = \nu / \alpha \) is the Prandtl number. Solutions to Eq. 5.27 were found here for various \( Pr \) via a finite difference (FD) method. Again, rather than utilizing tabulated data (now for each \( Pr \)
we sought a simple and compact function to approximate the temperature field arising from the solution to Eq. 5.27. The FD solutions to Eq. 5.27 were fit with a complementary error function

\[ \theta(x, y) \approx \text{erfc} \left( b(Pr) \sqrt{\frac{U_\infty}{2\nu x}} \right) \]  \hspace{1cm} (5.28)

where \( b \) is the parameter adjusted to fit Eq. 5.28 to the FD solutions of Eq. 5.27 for each \( Pr \). Since the \( b \) parameter in Eq. 5.28 essentially scales the thermal boundary layer thickness, it is expected to preserve the classical dependence with \( Pr \). Namely, the ratio of the thermal boundary layer thickness to the hydrodynamic boundary layer thickness should be proportional to \( Pr^{-1/3} \) \[16,18\]. Evidence of the scaling of \( b \) with \( Pr \) can be seen in Figure 5.4, and thus, the fitting function for the temperature field takes the form

\[ \theta(x, y) \approx \text{erfc} \left( 0.4542 Pr^{1/3} \sqrt{\frac{U_\infty}{2\nu x}} \right) \]  \hspace{1cm} (5.29)
To impose the required boundary conditions on the LBM framework (hydrodynamics), a variety of methods were employed. The no-slip and uniform inflow boundary conditions were achieved through use of the bounce-back method of [13]. The free slip and outflow boundary conditions were completed by way of the anti-bounce-back method [19] and extrapolation [20, 21], respectively. The constant temperature boundary at the inflow ($T_0$) was achieved by specularly reflecting all tracers that cross the boundary and setting their tracer type to 0. The constant temperature at the bottom wall ($T_1$) was achieved in the same manner, except tracers were set to type 1. The adiabatic boundary was achieved by merely specularly reflecting all tracers reaching the boundary without altering their types. The outflow boundary was achieved by imposing Eq. 5.14 on all tracers that reach the outflow plane. Tracers that vacated the domain were randomly re-seeded at the inflow plane and their types were set to 0. The inflow velocity and kinematic viscosity were fixed for all simulations while the thermal diffusivity was varied to achieve different $Pe$ and $Pr$ numbers. A summary of the simulation conditions may be found in Table 5.1.
Table 5.1: Simulation inputs for flow past a hot plate.

<table>
<thead>
<tr>
<th>Geometry and Operating Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>LBM Space</strong></td>
</tr>
<tr>
<td>Number of Nodes</td>
</tr>
<tr>
<td>$C_t$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physical Space</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Hydrodynamic Properties (fixed)</strong></td>
</tr>
<tr>
<td>$U_\infty$</td>
</tr>
</tbody>
</table>
| $
u$                             | $1.0 \times 10^{-5} \, [m^2/s]$ |
| $Re$                             | 1750                         |

<table>
<thead>
<tr>
<th><strong>Thermal Properties (varied)</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$</td>
</tr>
<tr>
<td>Pr</td>
</tr>
<tr>
<td>$\alpha$</td>
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<td>Pr</td>
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</tbody>
</table>

5.6 Results

The dimensionless temperature ($\theta = C_1(r,t)/C_t$) and dimensionless tracer concentration ($\theta_t = (C_1(r,t) + C_0(r,t))/C_t$) obtained from RWPT are observed to display the qualitatively correct behavior; see Figure 5.5. Specifically, $\theta_t$ remains homogenous throughout the entire domain, particularly near the outflow boundary (plane at $X_{LBM} = 350$), while the temperature field ($\theta$) displays a growth in the thermal boundary layer as the distance from the leading edge is increased.

To quantitatively compare with BL theory, the streamwise velocity at the outflow plane ($X_{LBM} = 350$) was compared with Eq. 5.27, see Figure 5.6. While the velocity field obtained via LBM displays some similarities with the BL solution, there are significant quantitative and
Figure 5.5: (top) The dimensionless total tracer concentration and the (bottom) dimensionless temperature extracted from RWPT for $Re = 1750$, $Pr = 0.2$.

qualitative differences. Namely, the LBM velocity field shows a compression of the hydrodynamic BL (defined as 99% of free-stream velocity) as well as non-monotonic behavior as the free stream velocity is approached. These effects can be attributed to the fact that LBM solves the full NS equations while Eq. 5.25 is a product of solving the Prandtl equations. The compression of the hydrodynamic BL and non-monotonic behavior are physical and a result of higher order BL effects [22, 23] not accounted for in the Prandtl equations.
Figure 5.6: The dimensionless stream-wise velocity extracted at the outflow plane \((X_{\text{LBM}} = 350)\) from LBM compared to the BL solution.

Similarly, the temperature field \((\theta)\) at the outflow plane was compared with Eq. 5.29; see Figure 5.7. For all \(Pr\) considered here, the temperature field obtained via RWPT is in reasonable agreement with the thermal BL solution - i.e., the temperature field monotonically decays as the distance from the bottom plate is increased and the thermal BL compresses with increasing \(Pr\). Therefore, the semi-reflecting barrier given by Eq. 5.14 is observed to achieve a fully developed outflow BC over a wide range of \(Pe\) and \(Pr\) that is similar to the analytical approximation obtained from BL theory.
A technique is presented here for imposing a fully developed outflow boundary condition on a RWPT algorithm that has been coupled to a hydrodynamic solver. A semi-reflecting barrier was developed by utilizing a mirror image of the near boundary region, coupled with $\frac{\partial u}{\partial n} = 0$ already being imposed upon the hydrodynamic field. Analytical means were utilized to calculate the probability of a tracer being specularly reflected back into the domain. The probability of being reflected has a dependence upon the $Pe$ and recovers the classic adiabatic boundary in the limit that $Pe \to 0$. The semi-reflecting barrier was implemented within a hybrid LBM-RWPT framework and utilized to simulate flow past a hot plate. Outputs from the LBM-RWPT method were compared to BL theory and show that the semi-reflecting barrier achieves a fully developed outflow over a wide range of $Pe$ and $Pr$. The differences between LBM-RWPT and BL theory can
be attributed to the simplifying assumptions made in BL theory (Prandlt equations) that are not present in LBM (Navier-Stokes equations).

The changes made to the DNS code in Chapter 4 permitted the simulation of interphase heat transfer between mediums with different thermal properties. Here, general means for imposing an outflow boundary condition are derived and verified for wall-bounded flows. The combination of these two modifications gives LBM-RWPT the capability of simulating multiphase heat transfer in wall-bounded systems. Therefore, indirect conduction theory may be rigorously tested with the current DNS implementation. In Chapter 6, flow past a hot plate and static, cold particle will be simulated and outputs from DNS will be directly compared to indirect conduction theory.
5.8 Chapter 5 Bibliography


Chapter 6

Heat Transfer to a Particle in a Laminar, Thermal Boundary Layer

6.1 Abstract

In many industrial systems, bounding walls or immersed surfaces are utilized as the primary thermal source to heat a gas-solids mixture. As a result, the heat transfer in the near-wall region is of great significance. To resolve the heat transfer near a boundary, convection correlations developed for unbounded systems (no walls) are extended into the near-wall region in conjunction with particle-scale models for indirect conduction. Here we rigorously test the unbounded convection correlations and indirect conduction models against outputs from direct numerical simulation of laminar flow past a hot plate and a static, cold particle. The unbounded convection correlations alone are found to under predict the heat transfer occurring in the near-wall region. While further incorporation of indirect conduction captures the first order physics associated with near-wall heat transfer enhancement, the conductive length scale commonly employed for indirect conduction is incorrectly identified as being proportional to the particle size. By contrast, it is observed that the key length scale associated with near-wall heat transfer enhancement is the thickness of the thermal boundary layer. An approximation of the thermal boundary layer thickness from classic boundary layer theory is utilized to develop a Nusselt correlation for the near-wall region. The new correlation accounts for both convection as well as indirect conduction and asymptotically decays to the unbounded convection correlation for large particle-wall separation distances, thereby seaming

---

together the unbounded and near-wall regions.

6.2 Introduction

The design and operation of various industrial processes is highly dependent upon the transport of thermal energy within a gas-solids flow. In many systems, domain walls or immersed surfaces are utilized as the primary energy source to heat a particle-laden mixture [1–13]. Under such conditions, the heat transfer occurring between a wall and a gas-solids flow will be of primary significance. Despite prevalent use of such flows in industry, fundamental explorations on wall-to-particle heat transfer have been largely unreported in the literature. While a variety of convective heat transfer correlations have been reported for unbounded gas-solids flows (no walls) [14–17], they inherently do not account for boundary effects. By and large, these unbounded correlations are directly extended into the near-wall region where their validity will deteriorate. On many occasions direct numerical simulation (DNS) has been employed to probe the heat transfer occurring within an unbounded gas-solids system [16–26]. However, works-to-date which account for wall-to-particle heat transfer (boundary effects) are far less inclusive [9, 27].

The heat transfer occurring between a particle and a wall is comprised of convective, conductive, and radiative mechanisms. For the case of moderate system temperatures ($T \leq 700K$), radiation is often neglected since it will not be a significant contribution to the overall heat transfer [28, 29]. Under these circumstances, the relevant heat transfer mechanisms may be simplified to convection and conduction only. Typically, correlations for unbounded systems [14–17] are utilized to approximate the interphase convection in the near-wall region. To account for conduction, particle-scale models have been largely relied upon. Specifically, the conduction occurring between a particle and wall is made up of two contributions: (i) direct conduction through the particle-wall contact area [30, 31] and (ii) indirect conduction between a particle and wall separated by a thin layer of fluid [32]. In many practical cases, indirect conduction tends to dominate over direct conduction - i.e., the ratio of thermal resistances associated with direct and indirect conduction is much greater than unity, or $\beta = R_p k_g \dot{h}_{FW}(0)/2 k_p R_c >> 1$, where $R_p$ is the particle radius, $k_g$
is the gas thermal conductivity, \( \dot{h}_{PFW}(0) \) is the solution to the indirect conduction integral at a particle-wall separation distance of zero \cite{33}, \( R_c \) is the radius of contact between the particle and wall, and \( k_p \) is the particle thermal conductivity. While the theory for indirect conduction is well established, with closures \cite{32,34,36} being utilized for a wide variety of systems \cite{1,4,37,40}, the particle scale models have not been validated. Most commonly, indirect conduction theory assumes that each particle is surrounded by a static fluid lens (\( R_{\text{Lens}} \)) (denoted by the dashed line in Figure 6.1). When the fluid lens overlaps the wall, one-dimensional conduction occurs through the fluid lens. Therefore, the fluid lens thickness is the key length scale that establishes distances over which particle-wall conduction will occur - i.e., heat transfer in addition to the unbounded convection correlation. Recent work has highlighted the sensitivity of indirect conduction to the fluid lens thickness, as well as the fact that the fluid lens is traditionally set according to the particles size (\( R_{\text{Lens}} \propto R_p \)) \cite{33}. Therefore, the current state-of-the-art for modeling near-wall heat transfer involves the direct extension of unbounded heat transfer correlations into the near-wall region as well as the use of particle scale models (indirect conduction) which have not been rigorously tested. For gas-solids flows at moderate temperatures (dominated by convection and indirect conduction), further work is required to assess the accuracy of these methods in the near-wall region.
In the present work, we utilize a hybrid lattice Boltzmann - random walk (LBM - RWPT) based DNS code [41-44] to examine the heat transfer to a spherical particle in the near-wall region. The heat transfer to a static particle in a laminar, thermal boundary layer is considered here - i.e., uniform flow of a fluid past a hot plate and a static, cold particle. The presence of a hot wall in this work allows boundary effects on wall-to-particle heat transfer to be quantified. Particle heat rates obtained from LBM-RWPT are compared to the heat rates predicted by unbounded convection [14] and indirect conduction [32] closures commonly employed within the discrete element framework (DEM). The unbounded convection correlations alone are found to under predict the heat transfer to a particle in the near-wall region since they do not fundamentally account for the presence of the wall. By contrast, the combination of unbounded convection and indirect conduction is observed to agree much better with outputs from LBM-RWPT. Indirect conduction theory is observed to capture the first order physics associated with heat transfer enhancement in the near-wall region. However, heat transfer enhancement is observed in LBM-RWPT at particle-wall separation distances ($\delta$) not predicted by indirect conduction theory. Namely, indirect conduction theory sets the fluid lens thickness according to geometric arguments based upon the particle size ($R_{Lens} = 1.4R_p$)
and thus, predicts near-wall heat transfer will occur when the fluid lens intersects the wall \((\delta \leq 0.4R_p)\). However, setting the fluid lens thickness in this manner neglects the thermal length scale associated with the fluid near the wall (boundary layer thickness). By contrast, we find that the thermal boundary layer thickness \((\delta_T)\) associated with the wall is the correct length scale associated with heat transfer enhancement in the near-wall region. An approximation for \(\delta_T\) is utilized to develop a Nusselt number correlation in terms of the dimensionless separation distance \((\hat{\delta} = \delta/\delta_T)\). The Nusselt correlation is observed to asymptotically decay to the unbounded convection correlation in the limit of large \(\hat{\delta}\) (particle outside the thermal boundary layer), and thus, seams together the unbounded and near-wall regions. Furthermore, the developed correlation accounts for heat transfer to a particle due to both convection as well as indirect particle-fluid-wall conduction.

### 6.3 Background: Indirect Conduction Theory

To account for the indirect conduction occurring between a particle and wall, we employ the model proposed by Rong and Horio \[1, 32\]. In this theory, particles are assumed to be surrounded by a static fluid lens (dashed line in Fig. 6.1). When the lens overlaps with the wall, one-dimensional conduction through the fluid lens is assumed to occur between the particle and wall. Motivation for describing the fluid lens as static is guided by the effect of no-slip boundary conditions on the particle and wall. As the separation distance \((\delta)\) between the particle and wall becomes small, the interaction between the no-slip boundaries will result in fluid velocities, between the particle and wall, which are dramatically reduced from the free-stream velocity. The rate of heat transfer due to indirect conduction is found by integrating Fouriers law over the area of overlap between the fluid lens and wall:

\[
\dot{q}_{pfw} \equiv h_{pfw}[T_w - T_p] = \int_{r_{in}}^{r_{out}} \frac{2\pi k_p r}{\text{Max}(l, s)} (T_w - T_p) dr
\]  

(6.1)
\[ r_{in} = \begin{cases} \sqrt{R_p^2 - (s - R_p - \delta)^2} & \delta \leq s \\ 0 & \delta > s \end{cases} \]

\[ r_{out} = \begin{cases} \sqrt{R_p^2 - (R_p + \delta)^2} & \delta > \sqrt{R_{Lens}^2 - R_p^2 - R_p} \\ R_p & \delta \leq \sqrt{R_{Lens}^2 - R_p^2 - R_p} \end{cases} \]

where \( \dot{q}_{pfw} \) is the rate of heat transfer due to indirect conduction between the wall and particle, \( h_{pfw} \) is the particle-fluid-wall heat transfer coefficient, \( T_w \) is the wall temperature, \( T_p \) is the particle temperature, \( r \) is the radial position of the fluid lens overlap, \( l(r) \) is the conduction distance at a radial position of \( r \), \( s \) is the minimum conduction distance, \( \delta \) is the particle-wall separation distance, and \( R_{Lens} \) is the fluid lens radius. To evaluate the integral in Eq. 6.1 a fluid lens radius \( (R_{Lens}) \) and minimum conduction distance \( (s) \) must be specified. An upper bound for \( R_{Lens} \) is generally determined from geometric arguments and is given by \( R_{Lens} = \sqrt{2} R_p \approx 1.41 R_p \). Namely, the maximum fluid lens radius is set such that the upper bound of integration in Eq. 6.1 \( (r_{out}) \) does not exceed the particle radius at the point of solid body contact (\( \delta = 0 \)) - i.e., the conduction distance \( (l) \) remains well defined. The fluid lens radius utilized in this work matches that commonly employed in other works \( (R_{Lens} = 1.4 R_p) \) [1, 4, 33, 34, 40]. The minimum conduction distance \( (s) \) in Eq. 6.1 acts as a lower bound for the conduction distance \( (l) \). The minimum conduction distance can be physically interpreted as corresponding to either the size of surface asperities (roughness) or the mean free path of the gas (perfectly smooth). For the former case (rough), large-scale asperities on the surface of a particle or wall will result in finite separation distances even at contact. For the latter case (smooth), as the particle and wall tend to solid body contact (\( \delta = 0 \)), the conduction distance \( (l(r)) \) becomes small with respect to the mean free path of the gas and rarefaction effects become non-negligible. By setting the minimum conduction distance to the mean free path of the gas \( (2.75 \times 10^{-8}[m]) \) the integration in Eq. 6.1 avoids conduction lengths where rarefaction effects are significant. Here, the particle and wall will be assumed to be perfectly smooth and the separation distance \( (\delta) \) will be kept large with respect to the mean free path of the gas. Therefore, the lower bound of integration in Eq. 6.1 \( (r_{in}) \) will always be 0 in the present work. The integral
in Eq. [6.1] may be nondimensionalized and directly evaluated [33]:

\[
\hat{h}_{pfw} = 2\pi \left( 1 + \hat{\delta} \right) \ln \left[ \frac{\sqrt{1 - \hat{r}_{out}^2} - (1 + \hat{\delta})}{\hat{\delta}} \right] + \sqrt{1 - \hat{r}_{out}^2} - 1 \tag{6.2}
\]

\[
\hat{r}_{out} = \begin{cases} 
\sqrt{\hat{C}^2 - (1 + \hat{\delta})^2} & \hat{\delta} > \sqrt{\hat{C}^2 - 1} - 1 \\
1 & \hat{\delta} \leq \sqrt{\hat{C}^2 - 1} - 1
\end{cases}
\]

where \( \hat{\delta} \) denotes normalization by the particle radius, and \( \hat{C} = R_{Lens}/R_p = 1.4 \) is the fluid lens proportionality constant. The rate of heat transfer at a given dimensionless separation distance (\( \hat{\delta} = \delta/R_p \)) then becomes \( \hat{q}_{pfw} = k_g R_p h_{pfw}(\hat{\delta})[T_w - T_p] \).

6.4 Numerical Techniques

6.4.1 Lattice Boltzmann Method (LBM)

The DNS framework is a hybrid scheme based on two coupled methods. The first is the lattice Boltzmann method (LBM), which is utilized to resolve the fluid phase - i.e., solve the Navier-Stokes (NS) equations. The LBM scheme employed here matches that developed by Ladd and co-workers [47–49]. Due to a foundation in statistical mechanics, LBM discretizes the continuous Boltzmann equation rather than the NS equations. Since the Boltzmann equation governs the evolution of the molecular velocity distribution, LBM is concerned with discrete velocity distributions (population densities), as opposed to the hydrodynamic variables. The discrete velocity distributions are updated in this work according to the classic streaming and collision process:

\[
n_i(r + c_i \Delta t, \Delta t) \equiv n_i^*(r, t) = n_i(r, t) + \Omega_i(n(r, t)) \tag{6.3}
\]

where \( n_i \) is the discrete velocity distribution (population density of molecules at position \( r \) with a velocity \( c_i \)), \( \Delta t \) is the LBM time step (scaled to be unity), \( \Omega_i \) is the collision operator (a function of all the velocity distributions at a node \( n(r, t) \)), and \( n_i^* \) is the post-collision distribution function. The collision operator in this work is linearized about the local equilibrium state (\( n^{eq} \) and matches
that in [49]. The hydrodynamic quantities are given by the moments of the velocity distribution functions:

\[ \rho = \sum_i n_i \quad \mathbf{j} \equiv \rho \mathbf{u} = \sum_i n_i \mathbf{c}_i \quad \bar{\Pi} = \sum_i n_i \mathbf{c}_i \mathbf{c}_i \]  

(6.4)

where \( \rho \) is the density, \( \mathbf{j} \) is the momentum, and \( \bar{\Pi} \) is the fluid stress tensor. A first order Taylor expansion of the finite difference approximation in Eq. 6.3 followed by a Chapman-Enskog expansion shows that the LBM recovers the Navier-Stokes equations with the following closures for the shear (\( \eta \)) and bulk viscosities (\( \eta_b \)) [49]:

\[ \eta = -\rho c_s^2 \left[ \frac{1}{3} + \frac{1}{2} \right] \quad \eta_b = -\frac{2\rho c_s^2}{3} \left[ \frac{1}{\lambda_b} + \frac{1}{2} \right] \]  

(6.5)

where \( c_s^2 = 1/3 \) is the square of the speed of sound, and \( \lambda \) and \( \lambda_b \) are eigenvalues of the collision matrix. \( \lambda \) corresponds to the relaxation of the off-diagonal portion of the non-equilibrium stress tensor while \( \lambda_b \) corresponds to the relaxation of the diagonal portion of the non-equilibrium stress tensor. Coupling between the fluid phase and solid particles is completed by imposing a no-slip boundary condition at the particle surface. The net force and torque applied to a particle by the fluid is given by surface integration of the interphase momentum transfer (resulting from the no-slip boundary condition). While the particle in this work is held static, the force and torque may be utilized to find the new particle velocity and position (solid body mechanics). Particle collisions are treated via a hard sphere method (binary and instantaneous), though no collisions will occur in the present work.

### 6.4.2 Random Walk Particle Tracking (RWPT)

The second method within the DNS framework is random walk particle tracking (RWPT). RWPT is employed here to solve the advection-diffusion equation for thermal energy:

\[ \frac{\partial T}{\partial t} + \mathbf{u} \cdot \nabla(T) = \alpha \Delta(T) \]  

(6.6)
where $T$ is the thermal temperature and $\alpha$ is the thermal diffusivity. Similar to LBM, RWPT does not involve directly the continuum equation (Eq. 6.6 for RWPT), but instead RWPT monitors the positions of many tracers as they undergo displacement. The movement of each tracer depends upon the local velocity field obtained via LBM and as well as random fluctuations. An explicit time integration scheme is utilized within the present work to update the position of each tracer:

$$
\begin{align*}
\mathbf{r}_1(t + \Delta t) &= \mathbf{r}_1(t) + \mathbf{u}(\mathbf{r}_1, t)\Delta t + \xi(t)\sqrt{2\frac{\alpha_1}{\alpha_2}\Delta t} \left[ 1 - H\left(\zeta - \frac{\alpha_1}{\alpha_2}\right) \right] \\
\mathbf{r}_2(t + \Delta t) &= \mathbf{r}_2(t) + \mathbf{u}(\mathbf{r}_2, t)\Delta t + \xi(t)\sqrt{2\alpha_2\Delta t}
\end{align*}
$$

(6.7)

where $\mathbf{r}_i$ is the position of a tracer within phase $i$, $\mathbf{u}$ is the velocity at the tracer position before the step (found via trilinear interpolation of the LBM velocity field), $\xi$ is a random vector whose entries are sampled from a Gaussian distribution with zero mean and unit variance, $\alpha_i$ is the thermal diffusivity of phase $i$, $\Delta t$ is the random walk time step, $H$ is the Heaviside function, and $\zeta$ is a random number sampled from a uniform distribution on the span $[0, 1)$ ($\mathcal{U}(0, 1)$). Note that an inherent assumption in Eq. 6.7 is that the thermal diffusivity of phase 1 is greater than phase 2 ($\alpha_1 > \alpha_2$). In the present work, $\alpha_1$ will correspond to the fluid phase and $\alpha_2$ will correspond to the solid particle phase. The thermal temperature in RWPT is proportional to the local tracer concentration. In the present work, we impose a temperature gradient ($\Delta T = T_1 - T_0$) by utilizing two tracer types. Tracers labeled as type 1 correspond to the higher temperature ($T_1$) while tracers labeled as type 0 correspond to the lower temperature ($T_0$). The local temperature and dimensionless temperature are given as:

$$
T(\mathbf{r}, t) = T_1 \frac{C_1(\mathbf{r}, t)}{C_t} + T_0 \frac{C_0(\mathbf{r}, t)}{C_t}
$$

(6.8)

$$
\theta(\mathbf{r}, t) \equiv \frac{T(\mathbf{r}, t) - T_0}{T_1 - T_0} = \frac{C_1(\mathbf{r}, t)}{C_t}
$$

(6.9)
where \( C_1 \) is the concentration of type 1 tracers, \( C_0 \) is the concentration of type 0 tracers, \( C_t \) is the total tracer concentration of tracers in the domain, and \( \theta \) is the dimensionless temperature.

### 6.5 Systems Simulated

Uniform flow past a hot wall and a static, cold particle is considered; see Figure 6.2. Due to the presence of the hot wall, the steady-state fluid flow will be characterized by the development of a hydrodynamic and thermal boundary layer near the bottom plate. The center of the particle is located 5 particle diameters (\( D_p \)) away from the leading edge of the plate (\( L = 5D_p \)) in all simulations, while the particle-wall separation distance (\( \delta \)) and the particle Reynolds number (\( Re_{Part} \equiv |U_f - U_s|D_p/\nu = U_\infty D_p/\nu \)) are varied. The range for \( Re_{Part} \) is chosen to reflect common values observed in applications concerned with wall-to-particle heat transfer [1–13] and is given by \( Re_{Part} \in [1 \ 10] \). The range for \( \delta \) is chosen such that the particle resides completely within the boundary layer as well as completely outside the boundary layer and is given by \( \delta/R_p \in [0.01 \ 25] \). Since the distance from the leading edge (\( L \)) is fixed, the resulting plate Reynolds number (\( Re_{Plate} \equiv U_\infty L/\nu = 5Re_{Part} \); \( Re_{Plate} \in [5 \ 50] \)) will lie in the intermediate regime and the flow will be laminar (\( Re_{Plate} < \mathcal{O}(10^6) \)) [45]. The particle diameter and Prandtl number (\( Pr = \nu/\alpha \)) are fixed and set to 600\( \mu \text{m} \) and 0.7, respectively. The particle diameter is resolved by 10 LBM nodes (\( D_p/\Delta x_{LBM} = 10 \)) in all simulations. This resolution has been shown to reach the point of grid insensitivity for uniform flow past a particle at \( Re_{Part} = 40 \) [19], which is well above the largest \( Re_{Part} \) considered in this work. Furthermore, test simulations were conducted at a resolution of \( D_p/\Delta x_{LBM} = 20 \) and the resulting heat transfer coefficients differed from the \( D_p/\Delta x_{LBM} = 10 \) case by less than 1%. A complete overview of the simulation conditions is given in Table 6.1 while the fluid and particle properties are contained within Table 6.2.

To impose the required boundary conditions given in Figure 6.2, a variety of methods were employed. The hydrodynamic boundary conditions were imposed upon the LBM framework. Namely, the no-slip and uniform inflow boundary conditions were achieved via the bounce-back method [49]. The free slip and outflow boundary conditions were completed by way of the anti-bounce-
back method [50] and extrapolation [19, 51], respectively. The thermal boundary conditions were imposed upon the RWPT framework. Specifically, the constant temperature boundary at the inflow \( (\theta = 0.2) \) and bottom wall \( (\theta = 1) \) is achieved by a two-step process. First, all tracers that cross the boundary are specularly reflected back into the domain. Second, a number is sampled from \( U(0, 1) \). If the sampled value is less than or equal to \( \theta \), the tracer type is set to 1; else, the tracer type is set to 0. The constant particle temperature \( (\theta = 0) \) is achieved by setting all tracers that enter the particle to type 0. The adiabatic boundary is imposed by specularly reflecting tracers back into the domain (no alteration of type). The thermal outflow boundary is achieved by a semi-reflecting barrier [44]. If a tracer reaches the outflow plane, the probability of being specularly reflected back into the domain \( (P^*) \) is calculated as in [44]. A number is then sampled from \( U(0, 1) \), if the value is less than \( P^* \) the tracer is specularly reflected back into the domain, else the tracer is re-seeded at the inflow plane and its type is set according to the temperature boundary condition at the inflow plane \( (\theta = 0.2) \).
Figure 6.2: The geometry and boundary conditions utilized to simulate uniform flow past a hot plate (bottom wall in red) and a static, cold particle (blue sphere). The particle-wall separation distance ($\delta$) is the distance between the bottom of the particle and the wall (varied) while $L$ is the distance from the leading edge to the center of the particle (fixed).
Table 6.1: Simulation inputs for flow past a hot plate and a static, cold particle.

<table>
<thead>
<tr>
<th>Geometry and Operating Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mesh</strong></td>
</tr>
<tr>
<td>Nodes (x x y x z)  160 x 240 x 80</td>
</tr>
<tr>
<td>( \frac{D_p}{\Delta s_{LBM}} )  10</td>
</tr>
<tr>
<td>( C_t )  2.0</td>
</tr>
<tr>
<td>( L/D_p )  5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Simulation Conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Re(_{\text{Part}})</strong></td>
</tr>
<tr>
<td>1</td>
</tr>
<tr>
<td>2</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>6</td>
</tr>
<tr>
<td>8</td>
</tr>
<tr>
<td>10</td>
</tr>
</tbody>
</table>

Table 6.2: Simulation inputs for flow past a hot plate and a static, cold particle.

<table>
<thead>
<tr>
<th>Hydrodynamic and Thermal Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fluid Properties</strong></td>
</tr>
<tr>
<td>( \nu )  ( 1.570 \times 10^{-5} \frac{m^2}{s^2} )</td>
</tr>
<tr>
<td>( \alpha_1 )  ( 2.230 \times 10^{-5} \frac{m^2}{s^2} )</td>
</tr>
<tr>
<td>( k_f )  ( 2.624 \times 10^{-2} \frac{W}{mk} )</td>
</tr>
<tr>
<td>( Pr )  0.70</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Particle Properties</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_p )  600 ( \mu m )</td>
</tr>
<tr>
<td>( \alpha_2 )  ( 8.30 \times 10^{-7} \frac{m^2}{s^2} )</td>
</tr>
</tbody>
</table>
6.6 Results

In the present work, a hydrodynamic and thermal boundary layer will develop near the bottom wall and the extent to which the particle will interact with the boundary layer will depend upon the separation distance (δ); see Figures 6.3 - 6.4. For the case of a small separation distance (Fig 6.3 - 6.4 (left)), the particle is within the thermal boundary layer and will interact with the wall to a great degree. By contrast, for large separation distances (Fig 6.3 - 6.4 (right)), the particle is outside the thermal boundary layer and will have a small interaction with the wall. Due to the thermal source at the bottom wall, a spatially varying temperature field will be present (Fig. 6.4).

![Figure 6.3: The dimensionless stream-wise velocity (\(\hat{U}_x\)) profile for \(Re_{Part} = 10\) and a separation distance of (left) \(\delta/R_p = 0.2\) and (right) \(\delta/R_p = 10.0\). The white dashed lines indicate the location of the particle.](image-url)
Figure 6.4: The dimensionless stream-wise velocity ($\theta$) profile for $Re_{Part} = 10$ and a separation distance of (left) $\delta/R_p = 0.2$ and (right) $\delta/R_p = 10.0$. The white dashed lines indicate the location of the particle.

To quantify the heat transfer coefficient ($h$) or more generally the Nusselt number ($Nu = hD_p/k$) for a particle in the near-wall region, the relevant thermal driving force ($\Delta T$) must be defined. For the case of an unbounded system, such as in [14–17], the thermal driving force is taken to be the difference between the fluid temperature at the inflow plane ($T_{f,\infty}$) and the particle temperature ($T_p$) ($\Delta T = T_{f,\infty} - T_p$). In the present work, utilizing this definition for the thermal driving force will inherently neglect the effect of the wall temperature ($T_w$) and make the resulting $h$ values specific to the given simulation conditions. By contrast, the fluid temperature surrounding the particle ($T_{f,Loc}$) will be a product of both the inlet boundary condition ($T_{f,\infty}$) as well as the wall boundary condition ($T_w$). The local fluid temperature may be approximated by the integral of the fluid temperature ($T_f$), with respect to a weighting function ($g(r)$), over a spherical volume that surrounds the particle ($\Omega_y$) [18, 20]:

$$T_{f,Loc} = \frac{\iiint g(|r_y - r_p|) T_f(r_y) d\Omega_y}{\iiint g(|r_y - r_p|) d\Omega_y}$$  \hspace{1cm} (6.10)
where $T_f(r_y)$ is the fluid temperature, $g(r)$ is the weighting function, and $\Omega_y$ is the volume contained within a sphere of radius $2D_p$ whose center coincides with the particle center ($r_p$). As discussed in [20], the motivation for utilizing the given form of the weighting function ($g(r)$) is its consistency with techniques commonly employed to derive the volume-averaged equations of motion for a gas-solids mixture [52, 53]. Here, we define $\Delta T_{Loc} = T_{f,Loc} - T_p$ as the thermal driving force.

Physically speaking, as $\delta$ becomes large with respect to the wall boundary layer thickness (Fig. 6.3 (right)), the boundary effects on particle heat transfer will become negligible and the resulting Nusselt number should converge to those obtained for an unbounded system [14–17]. However, the Nusselt numbers obtained here will not converge to [14–17], even in the limit of $\delta \to \infty$, but this is solely due to using $\Delta T_{Loc}$ instead of $\Delta T$; see Figure 6.5. The disagreement between $Nu_{Loc}$ and [14–17] can be attributed to the interphase transfer of thermal energy that will cause $\Delta T_{Loc} < \Delta T$.

For the $Re_{part}$ considered here, the reduction in thermal driving force ($\Delta T_{Loc} < \Delta T$) causes the resulting Nusselt numbers to be 25-50% larger than those given in [14–17]. Specifically, the Nusselt numbers obtained using $\Delta T = T_\infty - T_p$ ($Nu_\infty$) agree with [14–17] while the Nusselt numbers obtained using $\Delta T_{Loc} = T_{f,Loc} - T_p$ ($Nu_{Loc}$) are larger than those given in [14–17].
Figure 6.5: Comparison between the Nusselt numbers for unbounded flow past a particle when the inlet fluid temperature ($N_u\infty$) (solid black dots) versus local fluid temperature ($N_uLoc$) (open dots) is utilized as the relevant driving force.

In the opposite limit of separation distance ($\delta \to 0$), a choice must be made in terms of the definition for $\Omega_y$. Since the radius of $\Omega_y$ is $2D_p$ (significantly larger than the particle), a subset of $\Omega_y$ will overlap with the wall ($\Omega_w$). For this case, the volume overlapping with the wall ($\Omega_w$) as well as the fluid volume ($\Omega_f$) was incorporated into the volume integration performed in Eq. 6.10 ($\Omega_y = \Omega_{f+w}$) and the temperature within $\Omega_w$ was set to the boundary condition temperature ($\theta = 1$). This choice was motivated by the interpolation techniques employed within the DEM framework [54]. In DEM, the thermal driving force is found by interpolating the fluid temperature to the location of the center of the particle. If a particle lies within a numerical cell adjacent to a wall, the interpolated fluid temperature will lie between the wall temperature ($T_w$) and the fluid temperature at the adjacent nodes. By including $\Omega_w$ into the calculation of $T_{f,Loc}$, the resulting values are more consistent with those achieved via interpolation techniques; see Figure 6.6. Neglecting $\Omega_w$ and only integrating over the fluid volume ($\Omega_y = \Omega_f$) will cause the resulting
$T_{f,\text{Loc}}$ to be reduced by 16-21%, and thus, the resulting heat transfer coefficients will increase. Ultimately, integration over the wall volume ($\Omega_y = \Omega_{f+w}$) was utilized in this work since it is a more conservative approach (results in smaller predicted $h$ values due to the larger thermal driving forces) and agrees better with interpolation of the fluid temperature.

Figure 6.6: The local, dimensionless fluid temperature ($\theta_{\text{Loc}}$) found via integration over $\Omega_{f+w}$ (solid lines) as well as integration over $\Omega_f$ (dashed lines) versus the dimensionless distance between the particle center and the wall ($\hat{r}_{p,y}$). Note, for $\hat{r}_{p,y} \geq 5$, $\Omega_y$ does not intersect the wall ($\Omega_w = 0 \rightarrow \Omega_y = \Omega_f$). The wall temperature ($\theta_w$) is included for reference.

For each LBM-RWPT simulation (Table 6.1), the heat rate to the particle ($\dot{q}$) and local fluid temperature ($T_{f,\text{Loc}}$) are extracted at steady state. The heat rates obtained from LBM-RWPT ($\dot{q}$) are directly compared to the convective ($\dot{q}_{\text{conv}}$) and indirect conduction mechanisms ($\dot{q}_{pfw}$) utilized in DEM. First, the unbounded convective correlation of $[14]$ ($\dot{q}_{\text{conv}} = h_{\text{conv}} A_p \Delta T_{\text{Loc}}$) is compared to LBM-RWPT; see Figure 6.7 (left). As the particle-wall separation distance becomes small, the heat transfer coefficient grows quite rapidly (note log x-axis) and the unbounded convection
correlation fails to characterize the heat transfer enhancement that occurs in the near-wall region. This behavior is expected since the correlation given in [14] (unbounded system) does not account for the thermal source associated with the boundary. Note that the dimensionless heat rate ($\hat{q}$) does not decay to unity as the separation distance becomes large. This behavior is solely a result of utilizing $\Delta T_{Loc}$ as the thermal driving force (see $N u_{Loc}$ in Fig. 6.5) and $\hat{q}$ would tend to unity if $\Delta T$ were utilized for the thermal driving force.

Inclusion of the indirect conduction mechanism [32, 33] into the DEM heat rate ($\dot{q}_{conv} + \dot{q}_{pfw} = h_{conv} A_p \Delta T_{Loc} + k_f R_p h_{pfw}(\delta)[T_w - T_p]$) is observed to agree markedly better with LBM-RWPT than the convection correlation alone; see Figure 6.7 (right). In contrast to the convection correlation, indirect conduction theory accounts for the effect of a boundary by assuming that one-dimensional conduction occurs through a stagnant layer of fluid between the particle and wall ($R_{Lens}$). However, heat transfer enhancement due to the hot wall is still observed at length scales not predicted by indirect conduction theory (peaks in Figure 6.7 (right)). The length scale for indirect conduction theory is the fluid lens thickness ($R_{Lens} - R_p$) and is set according to the particle size ($R_{Lens} = 1.4 R_p$) [33] - i.e., $\dot{q}_{pfw}$ only contributes to the total heat rate when $\delta < (R_{Lens} - R_p)/R_p = 0.4$ in Figure 6.7 (right).
Figure 6.7: (left) The heat rate obtained via LBM-RWPT ($\dot{q}$) normalized by the correlation ($\dot{q}_{conv}$) and (right) the sum of convection and indirect conduction theory ($\dot{q}_{conv} + \dot{q}_{pfw}$) versus dimensionless separation distance ($\hat{\delta}$).

Physically speaking, heat transfer enhancement due to the boundary should occur at a length scale associated with the thermal boundary layer thickness ($\delta_T$) of the plate, rather than the particle radius; see Figure 6.8. For example, if a particle that is large with respect to $\delta_T$ is considered (right particle in Fig. 6.8), the onset of indirect conduction (fluid lens just intersects the wall; $\delta = 0.4R_p$) would correspond to a particle outside the thermal boundary layer where the heat transfer is well approximated by the unbounded correlation alone. Thus, the heat transfer to the particle in this case would be over-predicted. By contrast, if a particle that is small with respect to $\delta_T$ is considered (left particle in Fig. 6.8), the onset of indirect conduction would correspond to a particle that is already encompassed by the boundary layer. In this case, the heat transfer to the particle would be under-predicted.
Figure 6.8: An illustration of particles (solid black lines) and their fluid lenses (dashed grey line) overlaid upon the scaling of the thermal boundary layer thickness ($\delta_T$). For particles small with respect to $\delta_T$ (left particle), the onset of indirect conduction occurs when the particle is inside the boundary layer. For particles large with respect to $\delta_T$ (right particle), the onset of indirect conduction occurs when the particle is outside the boundary layer.

Taking $\delta_T$ to be the key length scale, the heat transfer enhancement occurring in the near-wall region (Figure 6.7 (left)) is more generally interpreted as the interaction between the particle and the thermal boundary layer. From classic boundary layer theory for flow past a plate, $\delta_T$ may be approximated as $[45, 46]$

$$\delta_T \approx 5.0 \frac{x}{Re_{Plate}^{1/2} Pr^{-1/3}} \quad (6.11)$$

where $x$ is the distance from the leading edge ($5D_p$ in this work). The local Nusselt number for the unbounded system (open dots in Figure 6.5) may be approximated by the following line

$$Nu_{Loc} = 3.75 + 0.067 Re_{Part} \quad (6.12)$$
By utilizing $\delta_T$ as the key length scale and $Nu_{\text{Loc}}$ as the asymptotic limit for large particle-wall separation distances ($\delta \rightarrow \infty$), a compression of the LBM-RWPT data may be completed; see Figure 6.9. The data in Figure 6.9 is approximated by:

$$f_1(\hat{\delta}) = 1 + 0.8e^{260\hat{\delta}} + 0.53e^{-35\hat{\delta}} - 0.002e^{-0.5\hat{\delta}}, \text{or}$$

$$f_2(\hat{\delta}) = 1 + 1.13e^{-85\hat{\delta}}$$

(6.13)

where $\hat{\delta} = \delta/\delta_T$ is the dimensionless separation distance. Making use of Eqs. 6.12 - 6.13, the Nusselt number in the near-wall region then becomes

$$Nu = \frac{hD_p}{k_f} = f_i(\hat{\delta})Nu_{\text{Loc}}$$

(6.14)

where $f_i(\hat{\delta})$ is either $f_1(\hat{\delta})$ or $f_2(\hat{\delta})$ in Eq. 6.13. Since the heat transfer enhancement in the near-wall region grows rapidly as the separation distance becomes small ($\hat{\delta} \rightarrow 0$ in Fig. 6.9), the accuracy of the fitting function ($f_i(\hat{\delta})$) is again better illustrated on a log x-axis. Due to the larger number of fitting parameters, $f_1$ better characterizes the data. However, very reasonable accuracy is obtained with the reduced order $f_2$ function. Note that both $f_1$ and $f_2$ asymptotically decay to unity as $\hat{\delta} \rightarrow \infty$, which is the physically correct behavior ($Nu \rightarrow Nu_{\text{Loc}}$). The choice between $f_1$ and $f_2$ should be dictated by the desired accuracy. Therefore, the Nusselt correlation given by Eq. 6.14 seams together the unbounded and near-wall region while accounting for both convective and indirect conduction mechanisms. While the $f_i(\hat{\delta})$ fitting functions monotonically decay with increasing $\hat{\delta}$, the LBM-RWPT data displays a local minimum at $\hat{\delta} \approx 0.5$ that becomes more pronounced with increasing $Re_{Part}$. As $Re_{Part}$ increases, the thermal and flow length scales compress. By contrast, the volume element utilized to calculate $T_{\text{Loc}}$ remains constant (sphere of radius $2D_p$ in Eq. 6.10). Therefore, the spatial averaging in Eq. 6.10 begins to encompass regions of the hot boundary layer that are not significantly contributing to the particle heat transfer - i.e., $T_{\text{Loc}}$ is increased by averaging over hot fluid near the bottom wall that will tend to be advected away as $Re_{Part}$ increases.
Unfortunately, the formal accuracy of indirect conduction models in a generic system cannot be deduced from the present work. However, by identifying the thermal boundary layer thickness as the key length scale, some general trends may be noted. For particles that are large with respect to $\delta_T$ (right particle in Fig. 6.8), the current indirect conduction models within DEM are expected to over-predict the heat transfer to the particle. This can be traced back to the violation of the static-fluid lens assumption over a length scale of $0.4R_p$. Note that the boundary layer thickness can vary spatially and will compress with increasing Reynolds and Prandtl number. For the case of a particle that is small with respect to $\delta_T$ (left particle in Fig. 6.8), the current indirect conduction models are expected to under-predict the heat transfer to the particle. Namely, the particle will already be well within the boundary layer (where heat transfer enhancement occurs) at the onset of indirect conduction ($\delta \leq 0.4R_p$).

Figure 6.9: The Nusselt number obtained via LBM-RWPT normalized by the local Nusselt number (open dots in Figure 6.5) versus the non-dimensional separation distance on a logarithmic axis.
6.7 Conclusions

Direct numerical simulation was utilized to examine the effect of a hot boundary on heat transfer in a gas-solids mixture. The heat transfer to a static particle in a laminar, thermal boundary layer was considered. The heat rate obtained via LBM-RWPT shows that Nusselt correlations developed in unbounded systems (no walls) are not sufficient in the near-wall region while the combination of unbounded convection and indirect conduction is observed to agree markedly better with DNS. Indirect conduction theory can thus be interpreted as capturing the first order physics associated with heat transfer enhancement in the near-wall region.

While indirect conduction captures some of the physics associated with near-wall heat transfer, the length scale associated with near-wall heat transfer enhancement is found to be proportional to the thermal boundary layer thickness and not the particle radius (utilized by indirect conduction theory). The thermal boundary layer thickness and local Nusselt number (unbounded system with local fluid temperature as the driving force) are utilized to compress the LBM-RWPT data and develop a new correlation which is valid in the near-wall region. The new correlation asymptotically decays to the unbounded convection correlation in the limit of large particle-wall separation distance, and thus, seams together the unbounded and near-wall regions.

While not considered here, the particle(s) may translate in space as well as rotate (angular velocity). Furthermore, the diameter of the particle, distance from the leading edge, Prandtl number, and thermal wall boundary condition may be altered. The impact of each parameter on particle heat transfer is not known a priori but will be the subject of future work - i.e., testing the robustness of the present relation for Nu.
6.8 Chapter 6 Bibliography


Chapter 7

Summary and Future Work

7.1 Conclusions

Heat transfer in particle-laden flows is ubiquitous in many modern industrial operations. Most recently, solid particles have been considered for use as a heat transfer medium in novel designs for concentrated solar plants (CSPs) [1-3]. These particle-based CSP operations show great potential for providing sustainable and cost effective renewable energy. Thus, accurate predictions of the macro-scale heat transfer in particle-based systems is important to not only optimization of current industrial processes but to the design of new novel solar receivers. Heat transfer in the majority of the systems considered here are dictated by boundary effects, and thus the accurate prediction of wall-particle heat transfer is of primary significance. To date, the state-of-the-art approach for simulating heat transfer in wall-bounded systems involves the utilization of unbounded convection correlations (developed for systems without walls) and untested particle-scale models (indirect conduction). The simplifications made by state-of-the-art techniques draws into question their ability to accurately characterize the heat transfer within a near black body (NBB) receiver. A bottom up approach is taken here assess the current state-of-the-art as well as propose new fundamental models for wall-bounded heat transfer in gas-solids flows.

To begin with (Chapter 2), state-of-the-art techniques for wall-to-particle (indirect and direct conduction) were first implemented within a discrete element method (DEM) solver. The DEM framework is utilized to simulate the heat transfer within a NBB receiver. Additionally, a novel constant total heat flux boundary condition for multiphase flows was developed to better char-
acterize the NBB reciever. Previous treatments for a constant heat flux boundary in multiphase systems required that a heat flux be specified to each phase and lead to non-physical behavior (e.g., multiple wall temperatures). By contrast, the new boundary condition developed here fixes the total heat flux, yields a single wall temperature, and utilizes the local hydrodynamics to determine the heat flux to each phase. The new boundary condition was tested in four NBB receiver geometries and outputs from DEM show the physically correct behavior at the boundary. The simulations completed here also highlight the fact that the solids heat transfer strongly governs the NBB wall temperatures and that indirect conduction is the primary contribution to the solids heat flux. Therefore, the accuracy of the NBB wall temperatures, and thus the longevity of the design, will be dictated largely by the accuracy of indirect conduction theory.

As noted in Chapter 2, the wall-particle heat transfer will be strongly governed by the indirect conduction mechanism. However, the sensitivity of indirect conduction to its theoretical inputs had not been considered for a dynamic, multi-particle system. Additionally, indirect conduction theory requires two theoretical input parameters: fluid-lens thickness and minimum conduction distance. While the minimum conduction distance has stringent physical interpretations, the same cannot be said for the fluid lens thickness. Namely, the fluid lens thickness is traditionally set according to geometric arguments related to the particle radius. In Chapter 3, it is shown, for the first time, that indirect conduction theory is most sensitive to the fluid lens thickness and that the fluid lens thickness has no strict physical interpretation. Therefore, further investigation into the validity of indirect conduction theory is warranted and unambiguous means for setting the fluid lens thickness are of great practical significance.

Sensitivity analyses illustrate the sensitivity of indirect conduction theory to the fluid lens thickness input parameter (Chapter 3), and thus, the need for wall-particle heat transfer correlations based on first principles was highlighted. The highly-resolved Direct numerical simulation (DNS) must be employed to develop such correlations and test indirect conduction theory. However, the DNS method employed here first required development in order to faithfully reproduce the inter-phase heat transfer between fluid and particles (Chapter 4). Namely, challenges arising in the
random walk framework due to the presence of a discontinuous thermal diffusivity field (e.g., fluid and particle with different thermal diffusivity) were overcome via an interfacial tracer balance. The new random walk particle tracking algorithm was used to simulate particle-fluid heat transfer and the new scheme is shown to replicate the heat transfer occurring in high Biot number systems.

In addition to the complications associated with the discontinuous diffusivity field (Chapter 4), a new outflow boundary condition was necessary to simulate the wall-bounded flows that are relevant to the present work. Namely, the presence of a no-slip wall results in regions at the outflow plane that range from diffusion dominated (small Peclet number) to advection dominated (large Peclet number). Previous works have only quantified boundary conditions for the random walk method in the limit of complete diffusion or advection dominance. By contrast, a general method for imposing a fully developed outflow boundary on the random walk method is derived in Chapter 5. The outflow boundary is characterized by a semi-reflecting barrier in which tracers are either allowed to vacate the domain or are reflected back into the simulation domain. Outputs from DNS are verified against boundary layer theory and the new boundary condition is shown to depend upon the Peclet number, with asymptotic convergence to an open and impenetrable boundary in the limit of infinite and zero Peclet number, respectively.

The development of a novel multiphase DNS framework with heat-transfer (Chapters 4-5) allowed the wall-bounded flows relevant to particle-wall heat transfer to be investigated. Here (Chapter 6), DNS simulation of flow past a hot plate and static, cold particle is conducted. The heat rate outputs from DNS are compared to both unbounded convection correlations and indirect conduction theory. It was found that indirect conduction theory is a good first-order approximation for near-wall heat transfer. However, for the first time, necessary corrections to the indirect-conduction theory are found. Specifically, the near-wall heat transfer enhancement is observed to correspond to length scales associated with the thermal boundary layer thickness of the wall, rather than the particle radius (state-of-the-art for indirect conduction theory). In addition, a new convection correlation for use in DEM is developed here that is valid for the near-wall region and incorporates indirect conduction mechanisms.
7.2  Recommendation for Future Work

7.2.1  Analytical Scale up of Near-Wall Heat Transfer Coefficient

In Chapter 6, a novel convection correlation was developed for particle heat transfer in the near-wall region. The closure obtained for the Nusselt number compression (Eq. 6.14) is for a single particle and still retains an explicit dependence upon the dimensionless separation distance ($\hat{\delta}$). For a continuum description for the solids phase (i.e., TFM), discrete particles are not resolved, and thus, the separation distance of each particle is no longer known. In order to describe the heat transfer coefficient in a continuum framework, a coarsening of the single particle Nusselt number must be completed. Namely, the averaging methods employed in Chapter 3 that made use of the particle-wall distribution function (Eq. 3.3) may be extended to the single-particle Nusselt number obtained in Eq. 6.14. Unfortunately, the particle-wall distribution functions employed in Chapter 3 (Eqs. 3.4 - 3.8) are only valid for $\delta \leq 0.4R_P$, since that is the span over which they were extracted from DEM. If DEM was utilized to close the particle-wall distribution function over larger separation distances ($\delta \leq \delta_T$), the coarsening of Eq. 6.14 takes the same form as Eq. 3.3. The new continuum Nusselt number would retain only a dependence upon the solids volume fraction ($\epsilon_s$), and thus, could be readily implemented within TFM. It should be noted though that the closure obtained via this method would act as an upper bound for particle-wall heat transfer since the single-particle Nusselt number (Eq. 6.14) does not account for particle shielding and/or the dipole induced on the thermal boundary layer thickness by the presence of other particles.

7.2.2  Direct Numerical Simulation Work

As noted at the end of Chapter 6, the DNS simulations did not account for the effects of many physically relevant parameters. First and foremost, the effect of translating and rotating particles (linear and angular velocity) was not accounted for. In Chapter 6, an inherent assumption of steady-state heat transfer was made for each particle-wall separation distance. By contrast, as particles move throughout the domain, they stream across fluid temperature gradients and experience a
temporally varying heat transfer coefficient. Furthermore, the Stokes number becomes a critical parameter for moving particles. The Stokes number physically characterizes the ratio of the time scale associated with particle motion to the time scale of the fluid flow. For a small Stokes number, the inertia of the particle is negligible and the particle rapidly relaxes to the fluid velocity (i.e., the particle will trace out the fluid streamlines). For a large Stokes number, the inertia of the particle is significant and the particle will relax to the fluid velocity very slowly. To account for particle motion, the present LBM-RWPT code requires modification to account for the propagation of the particles over the tracer field - i.e., tracers are held stationary when the particle position is updated. In addition, the effects of multiple particles, particle size, varying leading edge distances, larger Reynolds numbers, and the Prandtl number was not accounted for in Chapter 6. Modification of the aforementioned properties within LBM-RWPT is straightforward and were not addressed solely due to time constraints.

7.2.3 Incorporation of Heat Transfer in the Collision Integral

While high-fidelity methods are of value when a large degree of accuracy is required, coarse-grained approximations are sufficient for many considerations. For lower accuracy requirements and/or larger systems, the two-fluid model is the framework of choice, owing to significantly faster process times (lower computational overhead). However, the representation of the effective conductivity for the solids phase still requires significant work. Namely, the empirical closures developed for packed or mildly agitated beds vary by an order of magnitude (depending upon the closure utilized) [4, 5]. Furthermore, the effective conductivity does not display a particle size dependence (reported vastly in the literature) and disagrees significantly with predictions made by DEM [6]. In contrast to the solids hydrodynamics, little progress has been made by extending kinetic theory to the solids heat transfer. To date, only the effect of streaming type mechanisms have been accounted for by kinetic theory - i.e., the likelihood of a particle to translate across thermal gradients (proportional to the fluctuating velocity). Therefore, the heat transfer between colliding particles has not been accounted for by modern kinetic theory. Since indirect conduction accounts for the
majority of heat transfer in many gas-solids systems (i.e., $\beta = R_p k_g / R_c k_p >> 1$), it is a natural candidate for inclusion in the kinetic theory collision term. Physically speaking, as two colliding particles become close to one another they undergo heat transfer (indirect conduction) that will act to relax their temperatures to an equilibrium temperature (characterized by the density and heat capacities of the particles). Since indirect conduction occurs between particles at finite separation distances (fluid lens thickness), it is consistent with the assumptions made by kinetic theory (binary and instantaneous collisions) and may be included within the collision integral present in the Boltzmann equation. Since particle-particle heat transfer will only occur if there is a thermal gradient, the fluctuating thermal temperature will likely play a key role, and thus a balance will likely need to be developed for this quantity (analogous to the granular temperature balance).
Complete Bibliography


Stefan Radl, Federico Municchi, and Christoph Goniva. “Near-wall effects for momentum, heat and mass transport in gas-particle suspensions at moderate Reynolds numbers”. In:


