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Modeling of heat transfer and reactive chemistry for particles in gas-solid flow utilizing continuum-discrete methodology (CDM)

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**Modeling of heat transfer and reactive chemistry for particles in gas-solid flow
utilizing continuum-discrete methodology (CDM)**

Jordan M. H. Musser

**Dissertation submitted to the Eberly College of Arts and Sciences
at West Virginia University
in partial fulfillment of the requirements
for the degree of**

**Doctor of Philosophy
in
Mathematics**

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particle heat transfer**

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Abstract

Modeling of heat transfer and reactive chemistry for particles in gas-solid flow utilizing continuum-discrete methodology (CDM) by Jordan M. H. Musser

A comprehensive multi-phase flow model requires coupled hydrodynamics, boundary conditions, heat and mass transfer, and chemical reaction kinetics. A model must also capture the multi-scale nature of these problems. Computational fluid dynamics-discrete element method (CFD-DEM) provides an accurate description of chemical reactions and heat and mass transfer at the particle scale. Currently, MFIX-DEM, the existing CFD-DEM used as the foundation for this work, can only model coupled hydrodynamics. This dissertation extends the functionality of MFIX-DEM by addressing the remaining deficiencies in three separate efforts.

The first effort outlined in this dissertation focuses on the algorithmic development of discrete mass inflow and outflow boundary conditions. This approach allows for the construction of more dynamic models of gas-solid systems. It permits the amount and type of particles to fluctuate during a simulation. Examples illustrating the added functionality are provided.

The second investigation explores the three modes of heat transfer in gas-solids systems. Models for particle-particle contact conduction, particle-fluid-particle conduction, particle-gas convection, and particle-particle radiation are selected. Model selection is based on model simplicity, acceptance in existing CFD-DEM heat transfer models, extendibility to particles of different sizes, and computational expense. Modifications are made to selected models before implementing them into MFIX-DEM. The implementation of each model is verified for simple two particle test cases, or in the case of gas-particle convection, a single fixed particle in a flowing gas. Strong agreement is observed between the simulation data and the analytic or numerical solution.

Finally, a mathematical interface for managing user-defined particle-gas chemical reactions is developed. The shrinking, unreacted core model is selected as the particle reaction model for its accurate physical account of particle-gas reactions and ability to allow particles to initially contain inert material. The implementation of the reactive chemistry interface is verified for a single reacting particle. Strong agreement is observed between simulation data and the analytic solutions for the particle's mass, species mass fraction, and internal energy equations. Agreement between the simulation data and analytic solution for the shrinking, unreacted core is considered acceptable.

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Nomenclature

A_{BC}	cross-sectional inlet area
A_c	contact area between two colliding particles
A_n	coefficients of Fourier series solution
A_s	surface area of a particle
Bi	Biot number
Bi'	Biot number associated with collision duration
C_A, C_B	concentration of species A and B
C_{pg}	gas phase specific heat
C_{pp}	particle specific heat
d	thickness of laminar sub-layer surrounding the indexed particle
D_{gn}	gas phase species n diffusion coefficient
D_m	diameter of particles belonging to solids phase m
D_{max}	maximum diameter of incoming particles over all solids phases
E^*	effective Young's modulus of two particles
E_b	rate of at which radiation is emitted from a black body
$Err_{v_{test}^i}$	error between user-provided and computed bulk density values
$\mathbf{F}_c$	total force resulting from collisions acting on a particle
F	shape (or view) factor for radiative heat transfer
$\mathbf{F}_{nc}$	total force not associated with collisions acting on a particle
F_p	placement frequency of incoming particles
Fo_p	Fourier number for a particle
Fo_p'	Fourier number for a collision
g_i	i^{th} component of the gravity vector
$\mathbf{g}$	gravity vector
$H^\circ(T_{REF})$	enthalpy of formation at reference temperature T_{REF}
H_A, H_B, H_C, H_D	enthalpies of species A, B, C, and D
$\dot{H}_{fr}$	enthalpy transfer due to mass transfer
I	mass moment of inertia
I_{gm}	interphase momentum transfer between the gas and the m^{th} solids phase
l_{BC}	length of inlet region
k	rate coefficient of a chemical reaction
K_{CV}	function used to distribute the point-form drag force to the Eulerian grid

k_n	normal spring coefficient
k_t	tangential spring coefficient
$L^{(i)}$	distance from the center to the point of contact of the indexed particle
$\ell^{(i,j)}$	distance between the centers of the particles indexed by i and j
$\ell^{(m)}$	length of m^{th} thermal pipe in the particle assembly
$\ell_{i,r}$	length of path of conduction through the i^{th} particle $\mathfrak{L}$
$\ell_{g,r}$	length of path of conduction through the gas
m^*	effective mass of two particles
m	mass of i^{th} particle
M	total number of solids phases
m_{sn}	species n mass of reactant initially in the indexed particle
m_{sn}^0	species n mass of reactant consumed in the indexed particle
M_g	molecular weight of the gas phase
N_{BC}	number of cells in the staging area of the inlet
N_{CV}	number of particles in the control volume, CV
N_g	number of species comprising the gas phase
$N_{m,t}$	number of solids phase m particles entering the system per unit time
N_p	number of particles in a simulation
N_{ps}	number of particles seeded into the staging area
$N_{p,\Omega}$	number of particles in radiation domain, Ω
N_s	number of species comprising the indexed particle
N_t	total number of particles entering the system per unit time
Nu_p	Nusselt number of a particle
p_g	gas pressure
Pr	Prandtl number
q_A	total heat flux across the surface of a type-A particle
q_c	thermal flux normal to the contact area of two particles
$\dot{Q}_{pfp}$	rate of heat transfer via particle-fluid-particle conduction
$\dot{Q}_{pg}$	rate of heat transfer via particle-gas convection
$\dot{Q}_{pp}$	rate of heat transfer via particle-particle conduction
$\dot{Q}_{rad}$	rate of heat transfer via particle-environment radiation
q_{gs}	rate of heat transfer between gas and solids phase
$\mathbf{q}_{\mathfrak{L}}$	heat flux of particle assembly $\mathfrak{L}$
R^*	effective radius of two particles
R	gas constant

R_c	radius of the circular contact region between two spheres
$\tilde{R}_c$	geometrically derived contact radius
R_f	distance delineating the upper bound of particle-fluid-particle conduction
R_{gn}	gas phase species n rate of production (or consumption)
r_g, r_s	distances delineating the region of particle-fluid-particle conduction
R_p	particle radius
Re	Reynolds number
$(-r_A), (-r_B)$	rates of disappearance of species A and B
r_C, r_D	rates of formation of species C and D
s	parameter that influences the total number of iterations used in identifying the uniform inlet velocity
$\mathcal{s}$	distance between the surfaces of the indexed particles
S_{gji}	gas phase stress tensor
t	time
t_c	particle-particle contact duration
$\mathbf{T}$	total torque forces acting on a particle
T_A, T_B	temperatures of type-A and type-B particles
T_g	temperature of the gas phase
$T_{g,\Omega}$	temperature of gas phase in radiation domain Ω
T_{Rg}	gas phase radiation temperature
$T_{\mathfrak{L}}$	temperature of particle assembly $\mathfrak{L}$
T_{env}	environment temperature surrounding a particle
t_p	time indicating next particle placement event
T_p	particle temperature
T_{p0}	particle initial temperature
$T_{p,ref}$	particle reference temperature
T_{REF}	reference temperature
$\mathbf{V}$	velocity of a particle
$\mathcal{V}_{CV}$	volume of a control volume (CV)
v_{gi}	i^{th} component of gas phase velocity
v_m^0	initial velocity for incoming particles of solids phase m
v_{min}	lower bound on incoming particle velocity
$\mathbf{V}_n$	normal relative velocity
v_{rand}	velocity delineating order and random placement of incoming particles

v_{test}^i	test velocity for incoming particles
$\dot{V}_m$	volumetric flow rate of solids phase m into the system
$\mathcal{V}_{CV}$	volume of control volume (CV)
$\mathcal{V}_p$	particle volume
$\mathbf{V}_t$	tangential relative velocity
w_{BC}	width of inlet region
$\mathbf{X}$	position of a particle
X_{gn}	gas phase's species n mass fraction
X_{pn}	indexed particle's species n mass fraction

Greek Symbols:

α, β	angles delineating the region of particle-fluid-particle conduction
α_k	polynomial coefficients for temperature dependent specific heat
β_m	local gas-solids momentum transfer coefficient
γ_{cp}	convective heat transfer coefficient for a particle
γ_{BA}	particle-particle convective heat transfer coefficient between particle types A and B
γ_{Rg}	gas phase radiative heat transfer coefficient
δ_{ij}	Kronecker delta
δ_n	magnitude of normal overlap
δ_t	tangential displacement
ΔH	heat of reaction
ΔH_Q	change in enthalpy due to temperature change
ΔH_{rg}	gas phase heat of reaction
ΔH_{rs}	indexed particle's heat of reaction
ΔT_p	temperature change of a particle over a solids time step of Δt_s
Δt_s	solids time step size
∇T	temperature gradient along indexed thermal pipe in particle assembly $\mathcal{Q}$
ϵ	radiation emittance
ϵ_g	gas phase volume fraction
ϵ_{sm}	solids phase m volume fraction
ζ_p	particle emissivity
η	non-dimensionalized radial position
η_n	normal damping coefficient

η_t	tangential damping coefficient
$\eta_{\mathfrak{L}}$	thermal resistance of particle assembly $\mathfrak{L}$
Θ	non-dimensionalized particle temperature
θ_0, θ_c	angles delineating the region of particle-fluid-particle conduction
κ_g	gas phase thermal conductivity
κ_p	particle thermal conductivity
κ_p^*	effective thermal conductivity
$\mathbf{\kappa}_{\mathfrak{L}}$	thermal conductivity of particle assembly $\mathfrak{L}$
$\bar{\kappa}_{\mathfrak{L}}$	uniform thermal resistance of all thermal pipes in particle assembly $\mathfrak{L}$
λ_n	eigenvalues of Fourier series solution
μ	friction coefficient
μ_g	gas phase viscosity
μ'_g	second coefficient of gas phase viscosity
ν	Poisson's ration
ξ	unit vector directed along the indexed thermal pipe
ξ_n	unit normal vector relating the particles' centers
ξ_t	unit tangential vector relating the particles' centers
ξ'_t	unit tangential vector relating the particles' centers corrected for prolonged contact
ρ	radiation reflectance
ρ_{bm}	bulk density on solids phase m
$\tilde{\rho}_{bm}(v_{test}^i)$	test bulk density value
ρ_c	unreacted core denisty
ρ_g	density of gas phase
ρ_p	particle density
ρ_{sm}	density of solids phase m
σ	Stefan-Boltzmann constant ($5.67 \times 10^{-8} W/m^2 K^4$)
ς	radiation absorbance
τ_{gij}	gas phase viscous stress tensor
ω	angular velocity of a particle
ψ	resistance of thermal pipe
$\psi_{\mathfrak{L}}$	thermal resistance for particle assembly $\mathfrak{L}$
Ω	domain defining environment for radiation effects

Fraktur Symbols:

$\mathfrak{A}$	the set of particles engaged in particle-particle heat transfer with particle i
$\mathfrak{B}$	the set of particles engaged in particle-fluid-particle heat transfer with particle i
$\mathfrak{L}$	the set of particles contained in a specific control volume (particle assembly)
$\mathfrak{L}_{N_c}$	number of particle-particle contacts in particle assembly $\mathfrak{L}$
$\mathfrak{L}_{N_p}$	number of particles in particle assembly $\mathfrak{L}$

Abbreviations and Acronyms

AB	Adams-Bashforth method
CDM	continuum discrete method
CFD	computational fluid dynamics
CV	control volume
DEM	discrete element method
DMIBC	discrete mass inflow boundary condition
DMOBC	discrete mass outflow boundary condition
DNS	direct numerical simulation
DPM	discrete particle method
DSMC	direct simulation Monte Carlo
EE	Eulerian-Eulerian
LBM	lattice-Boltzmann method
MFIX	Multiphase Flow with Interphase eXchanges
MPPIC	multiphase particle in cell
TFM	two-fluid method

Chapter 1: Introduction

Gas-solids systems are found in industrial food preparation, mineral processing, pharmaceutical production, energy generation, and chemical production setups as well as academic research laboratories world-wide. Applications range from co-current flow drying processes for food particles [1] to fluidized bed reactors for polyethylene production [2]. With such a large industrial dependence on gas-solids systems, it is imperative that they are fully understood. A greater understanding of the physical processes occurring within a gas-solids system may yield designs that are more cost effective, energy efficient, and environmentally friendly.

Traditionally, design, scaling, and optimization of gas-solids systems are guided by empirical models derived from experimental observations [3,4]. The development of these models requires a large investment in both time and capital while their predictive capabilities remain limited and unreliable [5]. Consequently, multiphase computational fluid dynamics (CFD) models are gaining in popularity for testing various design considerations [6] and predicting flow characteristics [7]. This physics-based approach provides greater modeling flexibility since it is rooted in the first principles of gas-solids dynamics [8].

There are two general methods for modeling gas-solids flows. Simulations that solve continuum conservation equations for both the gas and solids phases are termed Eulerian-Eulerian (EE) or two fluid methods (TFM). Simulations that manage distinct objects for the solids phase while continuum conservation equations are solved for the gas phase are called Lagrangian-Eulerian (LE) or continuum discrete methods (CDM).

CDMs encompass a wide range of models that resolve gas-solids flow characteristics at various length and time scales [5]. These techniques include direct numerical simulation (DNS), lattice-Boltzmann method (LBM), CFD-discrete element method (CFD-DEM), direct simulation Monte Carlo method (DSMC), and multiphase particle in cell (MPPIC) methods. Each approach leads to a trade-off between computational expense and modeling complexity. A brief overview of these methods is found in the book, *Multiphase Continuum Formulation of Gas-Solids Reacting Flows* by Pannala, Syamlal, and O'Brien [5]. The primary goal of this work is to further the modeling capabilities of an existing CFD-DEM. Section 1.1 provides an overview of this modeling technique so that the objectives of this work are defined more clearly.

1.1 CFD-Discrete element method (CFD-DEM)

CFD-DEM combines two different modeling techniques for simulating gas-solids flows. The gas phase is described by a set of conservation equations that are solved over a static grid, similar to single phase CFD. In contrast, the solids phase is described by a collection of discrete particles that obey Newton's laws of motion. Each particle is individually tracked and all particle-particle collisions are resolved. This method of solids modeling is termed the discrete element method (DEM) but often is referred to as the discrete particle method (DPM).

The original concept of the CFD-DEM is found in the pioneering work of Tsuji, Tanaka, and Ishida [9]. In their research, a simple gas phase model is coupled with a DEM to simulate plug flow in a horizontal pipe. Since then, the simulation capabilities of the CFD-DEM have advanced. Initial investigations strived to refine the gas phase model [10,11], while new developments continue to improve the coupling of the gas and solids

phases [12]. Some research groups have incorporated Van der Waals forces to simulate cohesion between particles [13,14] as well as the Saffman and Magnus lift forces [15]. Presently, there is a large effort to include particle scale heat transfer and reactive chemistry models [2,11,16,17,18,19,20,21,22,23]. Sections 1.1.1 and 1.1.2 present the mathematical models for the gas and solids phases employed by the current CFD-DEM. A brief discussion covering the physical interpretation of the equations' components is provided. The gas phase model is introduced first, followed by a presentation of the solids phase model.

1.1.1 Gas phase mathematical model

The gas phase model employed by the CFD-DEM in this work is based on the volume averaging method of Anderson and Jackson [24,25]. In this approach, continuum equations for the gas phase are derived from the point form Navier-Stokes equations by converting *point variables* (e.g., gas velocity) to *local mean variables* [8]. The transformation occurs by incorporating a weighting function when averaging point variables over a region (volume) in space. Regions are defined so that they are small in comparison to *macroscopic* changes in flow characteristics within the system, but large enough to contain many particles [26].

The governing equations presented below only contain the source and sink terms found in references [24,25,27]. *Constitutive relationships* needed to define various terms that arise during the derivation of the continuum equations (model closure) are obtained from the gas-solids flow theory outlined by Syamlal, Rogers, and O'Brien [27]. A complete review of all possible source and sink terms as well as the many constitutive relationships presented in the literature is beyond the scope of this work.

1.1.1.1 Gas phase conservation of mass (continuity equation)

The continuity equation (also referred to as the conservation of mass) for the gas phase is given in tensor notation in Equation (1-1). Here and throughout this document, ε_g is gas phase volume fraction, ρ_g is gas density, v_{gi} is the i^{th} component of gas velocity, and R_{gn} is the rate that species n of the gas phase is generated or consumed. The superscript over the summation, N_g , is the total number of species that comprise the gas phase. (For example, the composition of dry air at sea level by mass percent is approximately N₂: 75.52%, O₂: 23.15%, Ar: 1.28%, and CO₂: 0.046% [28]. A simplified model of air is described by a combination of nitrogen and oxygen resulting in $N_g = 2$.)

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g) + \frac{\partial}{\partial x_i}(\varepsilon_g \rho_g v_{gi}) = \sum_{n=1}^{N_g} R_{gn} \quad (1-1)$$

The physical interpretation of the components of Equation (1-1) are identified best in the context of a control volume (CV). For the following discussion, one can think of a CV as the unit cube. The first term on the left hand side of Equation (1-1) describes the rate at which mass accumulates within the CV. The second component expresses the rate at which mass is *convected* (transported) across the boundaries of the CV. The term on the right hand side specifies the rate of mass production/consumption in the CV of the various gas phase species.

For simulations that do not include chemical reactions or phase changes, the term on the right hand side is zero, otherwise a constitutive relationship is needed to specify this quantity. Since the rate of production/consumption is dependent on the chemical and/or physical processes modeled, no specific constitutive relationships are proposed in this section to maintain generality.

1.1.1.2 Gas phase conservation of momentum

The conservation of momentum for the gas phase is given in tensor notation in Equation (1-2). Here, S_{gij} is the gas phase stress tensor, g_i is the i^{th} component of the gravity vector, and I_{gmi} represents the exchange of momentum between the gas and the m^{th} solids phase in the i^{th} direction. The superscript over the summation, M , is the total number of *solids phases* present during a simulation. The term solids phase is used in this work to identify all the particles in a system that have the same density, ρ_{sm} , and diameter, D_m .

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g v_{gi}) + \frac{\partial}{\partial x_j}(\varepsilon_g \rho_g v_{gi} v_{gj}) = \frac{\partial}{\partial x_j}(S_{gij}) + \varepsilon_g \rho_g g_i - \sum_{m=1}^M I_{gmi} \quad (1-2)$$

The first term of Equation (1-2) represents the rate at which momentum increases within the CV. The second component indicates the rate at which momentum is transported out of the CV across its boundaries. The terms on the right hand side represent various sources and sinks of momentum within a CV. The first component accounts for viscous forces acting on the gas and is defined below. The second term accounts for gravitational effects acting on the gas. The last component indicates the amount of momentum that is transferred between the gas and m^{th} solids phases. This quantity is the result of several physical phenomena including the drag, pressure, Basset, Saffman, Magnus, and virtual mass forces [29,30]. Further definition of this term is reserved for Section 1.1.2 where it is presented in the context of the solids phase model.

The gas phase stress tensor is defined in Equation (1-3) as a combination of the gas pressure, p_g , and the viscous stress tensor, τ_{gij} . Here, δ_{ij} is the Kronecker delta. An expression (constitutive relation) for the viscous stress tensor is obtained by assuming the

gas is a *Newtonian fluid*. This assumption implies that the rate of deformation of a fluid element is proportional to the viscous stresses, defined in Equation (1-4). Here μ'_g is the second coefficient of viscosity for the gas phase which is taken as $\frac{2}{3}\mu_g$. Additional details about viscous forces and Newtonian fluids are covered in the classic fluid dynamics text by Batchelor [31].

$$S_{gij} = -p_g \delta_{ij} + \tau_{gij} \quad (1-3)$$

$$\tau_{gij} = \mu_g \left(\frac{\partial v_{gi}}{\partial x_j} + \frac{\partial v_{gj}}{\partial x_i} \right) + \mu'_g \left(\frac{\partial v_{gk}}{\partial x_k} \right) \delta_{ij} \quad (1-4)$$

1.1.1.3 Gas phase conservation of species mass

For simulations that include phase changes (e.g., evaporation) or reactive chemistry (e.g., combustion), one must account for the generation and/or consumption of the individual species that comprise the gas phase. This is done through solving a conservation equation for each species. For a gas comprised of N_g species, this results in N_g equations of the form shown in Equation (1-5). In this equation, X_{gn} represents the mass fraction of the n^{th} species of the gas (i.e., the ratio of the mass of species n in the CV to the total mass of the gas in the CV), D_{gn} is the diffusion coefficient of the n^{th} species of the gas phase, and as before, R_{gn} is the rate at which the n^{th} species of the gas phase is generated or consumed.

$$\frac{\partial}{\partial t} (\epsilon_g \rho_g X_{gn}) + \frac{\partial}{\partial x_j} (\epsilon_g \rho_g v_{gj} X_{gn}) = \frac{\partial}{\partial x_j} \left(D_{gn} \frac{\partial X_{gn}}{\partial x_j} \right) + R_{gn} \quad (1-5)$$

The first term on the left hand side of Equation (1-5) describes the rate at which the n^{th} species accumulates within the CV, and the second component indicates the rate

at which this species leaves the CV across its boundaries. The first term on the right hand side represents the rate at which the n^{th} species enters the CV as a result of *diffusion*. The second component specifies the rate at which the species is generated or consumed through chemical and/or physical processes. As in the continuity equation, no expression for R_{gn} is specified to preserve generality.

1.1.1.4 Gas phase conservation of internal energy

The conservation of internal energy for the gas phase in terms of the gas temperature is shown in Equation (1-6). Here, C_{pg} , T_g , and κ_g are the specific heat, temperature, and thermal conductivity of the gas, respectively; q_{gs} is the energy transferred between the gas and solids phases, ΔH_{rg} is the heat of reaction, γ_{Rg} is the gas phase radiative heat transfer coefficient, and T_{Rg} is the gas phase radiation temperature.

$$\varepsilon_g \rho_g C_{pg} \left(\frac{\partial T_g}{\partial t} + v_{gj} \frac{\partial T_g}{\partial x_j} \right) = - \frac{\partial}{\partial x_i} \left(-\kappa_g \frac{\partial T_g}{\partial x_i} \right) + q_{gs} - \Delta H_{rg} + \gamma_{Rg} (T_{Rg}^4 - T_g^4) \quad (1-6)$$

The first term on the left hand side of Equation (1-6) represents the rate at which thermal energy accumulates within the CV, while the second component indicates the rate at which thermal energy is transferred out of the CV across its boundaries. The first term on the right hand side is the gas phase conductive heat flux and is closed (defined) assuming Fourier's law of heat conduction. The second component indicates the heat transfer between the gas and the solids in the CV. A detailed description of this term is reserved for Section 3.4 of Chapter 3 where it is presented in the context of particle-gas convection. The third term is the heat of reaction and is the result of an endothermic (energy absorbing) or exothermic (energy creating) chemical reaction. Further explanation of this term is postponed until Chapter 4 where it is discussed in the context

of the mathematical interface for managing gas-solids reactions. The last component is described via a simplified model for radiative heat transfer in the gas phase.

1.1.1.5 Gas phase equations of state

In addition to the gas phase continuity and internal energy equations, specifying an *equation of state* establishes a relationship between the thermodynamic variables of density, pressure, temperature, and specific internal energy. The ideal gas law, shown in Equation (1-7), is used commonly in CFD for compressible fluids [32]. In this example, the density of the gas is defined by the gas constant R and the pressure p_g , molecular weight M_g , and temperature T_g of the gas, respectively. If the gas phase is assumed incompressible, then it is common to define the density of the gas as a constant value.

$$\rho_g = \frac{p_g M_g}{RT_g} \quad (1-7)$$

This concludes the outline of the equations governing the gas phase. The interested reader is directed to [29,33] for additional theoretical treatment of gas phase modeling for multiphase flows.

1.1.2 Solids phase mathematical model

The solids phase in the CFD-DEM is represented by a collection of discrete particles that obey Newton's equations of motion, shown in Equation set (1-8). In these equations, for a particle indexed by the superscript (i) , the variables m , $\mathbf{X}$, $\mathbf{V}$, $\boldsymbol{\omega}$ and I indicate the particle's mass, position, linear and angular velocities, and mass moment of inertia, respectively. $\mathbf{F}_c^{(i)}$ are the total forces resulting from particle-particle and particle-wall collisions, $\mathbf{F}_{nc}^{(i)}$ are the total forces not associated with collisions (i.e., gas-solids

interaction, cohesion, etc.) , and $\mathbf{T}^{(i)}$ is the total torque acting on particle i . Bold face font is used throughout this work to identify vector quantities.

$$\begin{aligned}\mathbf{V}^{(i)} &= \frac{d}{dt}(\mathbf{X}^{(i)}) \\ \left(m^{(i)}\mathbf{g} + \mathbf{F}_c^{(i)} + \mathbf{F}_{nc}^{(i)}\right) &= m^{(i)} \frac{d}{dt}(\mathbf{V}^{(i)}) \\ \mathbf{T}^{(i)} &= I^{(i)} \frac{d}{dt}(\boldsymbol{\omega}^{(i)})\end{aligned}\tag{1-8}$$

The first equation in set (1-8) defines the velocity of the particle as the time rate of change of the particle's position. The second equation is typically referred to as *Newton's Second Law of Motion* and relates the forces acting on a particle to the product of its mass and acceleration. The third equation, similar to the second, relates the rotational forces (torque) to the product of the particle's mass moment of inertia and angular acceleration.

1.1.2.1 Particle-particle collision model

There are two general approaches to manage collisions within the CFD-DEM [30]. The *hard-sphere model*, first introduced by Allen and Tildesley [34], assumes that particle-particle collisions are binary and instantaneous. Hard sphere models usually employ an *event-driven* algorithm to advance the particles' positions throughout a simulation. This type of algorithm results in a time step that is inversely proportional to the volume fraction of the system [35]. This can produce prohibitively small time steps in simulations where dense regions of particles may occur. Furthermore, enduring, multi-particle collisions may arise in dense regions of a system, violating the assumption that particle collisions are binary [35,36]. These limitations lead to the adoption of the *soft-*

sphere model for more complex simulations [37]. However, the interested reader is directed to references [30,34,38,39,40] for additional details about hard-sphere models.

The soft-sphere model uses mechanical spring, dashpot and slider elements to account for the elastic, damping and rotational forces generated during a collision. The total collision force is comprised of normal and tangential components which are the result of a small overlap of the colliding particles, as illustrated in Figure 1-1.

Figure 1-1: Schematic of the soft-sphere model that employs mechanical elements to simulate particle-particle and particle-wall collisions.

The normal force resulting from contact is given by Equation (1-9). The first term is the conservative (spring) force while the second term is the dissipative (damping) force. In this equation, k_n is the normal spring stiffness, δ_n is the magnitude of the normal overlap, ξ_n is the unit normal vector relating the particles' centers, η_n is the normal damping coefficient, and $\mathbf{V}_n$ is the relative normal velocity. The algebraic and geometric definitions for these variables are reserved for Appendix A.

$$\mathbf{F}_n^{(i,j)} = -k_n \delta_n \xi_n - \eta_n \mathbf{V}_n \quad (1-9)$$

A Coulomb-type friction law is used for the tangential force in Equation (1-10). The first portion is the force associated with static contact between two touching particles and contains conservative and dissipative components. The second element is the force

associated with frictional slip between the particles' surfaces. In these equations, k_t is the tangential spring stiffness, δ_t is the tangential displacement, η_t is the tangential damping coefficient, $\mathbf{V}_t$ is the relative tangential velocity, μ is the friction coefficient, and ξ'_t is the tangent unit vector corrected for prolonged contact. As before, the algebraic and geometric definitions for these variables are reserved for Appendix A.

$$\mathbf{F}_t^{(i,j)} = \begin{cases} -k_t \delta_t - \eta_t \mathbf{V}_t & \text{for } |\mathbf{F}_t| \leq \mu |\mathbf{F}_n| \\ -\mu |\mathbf{F}_n| \xi'_t & \text{for } |\mathbf{F}_t| > \mu |\mathbf{F}_n| \end{cases} \quad (1-10)$$

The total collision force acting on particle (i) is given by Equation (1-11). Here, $\mathfrak{C}$ represents the set of particles in contact with particle (i).

$$\mathbf{F}_c^{(i)} = \sum_{k \in \mathfrak{C}} (\mathbf{F}_n^{(i,k)} + \mathbf{F}_t^{(i,k)}) \quad (1-11)$$

The torque acting on particle (i) from contact with particle (j) is given by Equation (1-12). Here, $L^{(i)}$ is the distance from the center of particle (i) to the point of contact. The total torque on particle (i) is given by Equation (1-13).

$$\mathbf{T}^{(i,j)} = L^{(i)} \xi_n \times \mathbf{F}_t^{(i,j)} \quad (1-12)$$

$$\mathbf{T}^{(i)} = \sum_{k \in \mathfrak{C}} \mathbf{T}^{(i,k)} \quad (1-13)$$

The soft sphere model uses a traditional time step-driven algorithm to advance the particles' positions throughout a simulation. The step size needed for numerical stability is a function of the spring stiffness and is typically small [9]. Additional details about the soft-sphere model as well as the spring and damping coefficients are provided in references [35,41].

1.1.2.2 Particle-wall collision model

Particle-wall collisions are managed similarly to particle-particle collisions with additional complexity arising from the need to represent the wall [41]. This work uses artificial particles to act as the wall during a collision. When the surface of a particle initiates contact with a boundary plane (wall), an artificial particle of the same size is generated. The artificial particle is assigned the physical properties associated with the wall and placed across the boundary, opposite the colliding particle, outside the computational domain. This process is illustrated in Figure 1-2-(a). Once the forces generated from the particle-wall collision are calculated, the artificial particle is removed. After the position and trajectory of the colliding particle are updated, a new artificial particle is created if the colliding particle remains in contact with the wall. This procedure continues until the collision has evolved fully and the colliding particle is no longer in contact with the wall, as illustrated in Figure 1-2-(b). This method of modeling particle-wall collisions ensures that any normal forces generated during the collision are always perpendicular to the boundary plane.

Figure 1-2: (a) During a particle-wall collision, an artificial particle the same size of the colliding particle is generated to represent the wall. The artificial particle is placed opposite the colliding particle, outside the computational domain. (b) As the position and trajectory of the colliding particle change, the artificial particles are replaced by new artificial particles to ensure that normal forces remain normal to the boundary plane.

1.1.2.3 Gas-solids momentum transfer

Interphase momentum transfer is the result of several physical phenomena including the drag, Basset, Saffman, Magnus, and virtual mass forces [29,30,42]. This work assumes that gas-solids drag is the only significant interaction force between the gas and solids. Consequently, only the gas-solids drag term is presented below.

The gas-solids drag force acting on the particle indexed by (i) , belonging to solids phase m , and contained within the control volume (CV) is shown in Equation (1-14). Here, $\mathcal{V}^{(i)}$ is the volume of the particle $\left(\frac{4}{3}\pi(R_p^{(i)})^3\right)$, $p_g^{(i,CV)}$ is the gas phase pressure at the particle's position, ε_{sm}^{CV} is the solids volume fraction of the m^{th} solids phase in the CV, and $\mathbf{v}_g^{(i,CV)}$ is the gas phase velocity at the particle's position. $\beta_m^{(i,CV)}$ is the local gas-solids momentum transfer coefficient for particle (i) in the CV. Several expressions for $\beta_m^{(i,CV)}$ are available in the literature [42], therefore no specific model is presented here to preserve generality.

$$\mathbf{F}_{nc}^{(i)} = -\mathcal{V}_p^{(i)} \nabla p_g^{(i,CV)} + \frac{\beta_m^{(i,CV)} \mathcal{V}_p^{(i)}}{\varepsilon_{sm}^{CV}} \left(\mathbf{v}_g^{(i,CV)} - \mathbf{v}^{(i)} \right) \quad (1-14)$$

Equation (1-15) defines the corresponding force acting on the gas phase through the interphase momentum transfer term, $\mathbf{I}_{gm}$. Here, $\mathcal{V}_{CV}$ is the volume of the CV, N_m is the number of solids phase m particles contained in the CV, and $K_{CV}^{(i)}$ is a function used to distribute the point-form drag force to the computational nodes of the gas phase Eulerian grid.

$$\mathbf{I}_{gm} = \frac{1}{\mathcal{V}_{CV}} \sum_{k=1}^{N_m} \mathbf{F}_{nc}^{(k)} K_{CV}^{(k)} \quad (1-15)$$

This concludes the outline of the solids phase model. The interested reader is referred to [35,37,41,42] for additional information concerning the DEM and its implementation.

1.2 Dissertation objectives

Efforts to further enhance the CDM, with a strong emphasis placed on heat transfer and specific reactive chemistry models, are published in the literature [2,11,16,17,18,19,20,21,22,23]. The goal of this work is to add to this body of research by introducing three new modeling capabilities to an existing CFD-DEM:

1. develop discrete mass boundary conditions;
2. construct a mathematical description of particle scale heat transfer in the context of gas-solids flows; and
3. develop a generic mathematical interface to manage user-specified gas-solids chemical reactions.

MFIX-DEM (Multiphase Flow with Interphase eXchange), an open-source multiphase flow software package [27,43], is the CFD-DEM framework wherein all work

is conducted. Accordingly, all programmatic efforts follow the FORTRAN90/95 coding standard.

1.3 Document organization

Chapter 2 presents the algorithmic description of the discrete mass inflow and outflow boundary conditions. Details concerning the implementation of the boundary conditions into MFIX-DEM are discussed and two examples illustrating the behavior of the discrete mass inflow boundary condition are given. Chapter 3 begins by defining the three modes of heat transfer and the internal energy equation for a single, isothermal particle. An examination of the assumption of isothermal particles is conducted. In the subsequent sections, an analysis of contact conduction, particle-fluid-particle conduction, particle-gas convection, and particle-environment radiation are presented. Each investigation includes (1) a survey of models proposed for the specified mode of heat transfer, and (2) a discussion detailing modifications made to the selected model. Finally, the algorithmic implementation and verification of the selected heat transfer models are given. In Chapter 4, a discussion of reactive chemistry is presented in conjunction with a survey of previous efforts to incorporate reactive chemistry into the CFD-DEM. Then the mathematical interface for managing user-defined chemical reactions and its implementation into MFIX-DEM are outlined. Finally, a brief study verifying the interface is discussed. Finally, in Chapter 5 a summary of this work's efforts is presented along with areas of interest for future investigations.

Chapter 2: Discrete mass boundary conditions

In mathematics, boundary conditions, like those of Neumann and Dirichlet, are typically considered in the context of differential equations. However, in a discrete element model (DEM), there is no natural analogue to specify the flux of solids into a system. This investigation aims to develop a Neumann-like boundary condition algorithm for introducing new solids into a simulation that employs the DEM. This work also describes the construction of a mass outflow boundary region. The algorithms are termed the discrete mass inflow boundary condition (DMIBC) and discrete mass outflow boundary condition (DMOBC).

2.1 Introduction

Recall from Chapter 1 that the contact force scheme of Cundall and Strack [44] is adopted for this work. In their model, mechanical elements are used to account for the elastic, damping and rotational forces generated during a particle-particle collision. As particles collide, the deformation of each particle's shape is captured through an overlap of their contact regions. The magnitude of the overlap is related to the scale of the forces resulting from impact. As the collision evolves, the resultant forces are used to recalculate the positions, trajectories, and rotational speeds of the particles.

Since the overlap between particles is used to determine the kinetic response to a collision, a particle entering the system cannot be placed overlapping another particle. This limitation is apparent if a DMIBC is defined along a domain region that is associated with a high particle density, such as a packed bed. To avoid improper placement of particles while retaining the ability to define a DMIBC along any region of

the domain, a staging area is designated outside of the computational domain. This is illustrated in Figure 2-1.

Figure 2-1: The staging area for incoming particles is located outside of the computational domain, in the ghost cells bordering the region identified with the boundary condition.

Particles are seeded into the staging area and then incrementally moved across the boundary into the domain of the system. The behavior of the particles within the staging area is controlled so that given acceptable boundary condition parameters (discussed in Section 2.2.1), a new particle can be introduced to the staging area without overlapping previously inserted particles.

As a particle passes from the staging area into the computational domain, contact forces acting on the incoming particle are dismissed temporarily but particles already within the system respond accordingly. Thus, entering particles will move particles obstructing their entry out of the way, despite any disparities in size or density. Once an incoming particle has entered the domain fully, it then responds to any forces acting on it in complete accordance to the DEM. Here it is assumed that since there is a net flux of particles into the system and the solids fraction near the inlet region is relatively low (i.e.,

not packed) for most situations [45,46], the overall effect of incoming particles neglecting contact forces is negligible.

An outflow boundary condition for the DEM results in a modification of the particle-wall collision algorithm. In its application, when a particle collides with a wall region associated with an outlet, the collision force is ignored. This allows the particle to move from the computational domain to a bordering ghost cell over a series of time steps. Once the particle has exited the computational domain fully, all instances of the particle are removed from memory.

2.2 DMIBC algorithm description

The DMIBC has two operating components. The first element is called during the initialization of the software, wherein user provided data is checked for consistency, and operational characteristics are determined. The second element is executed during the simulation, and controls the placement and assignment of physical properties to incoming particles. The two components of the algorithm are outlined below.

2.2.1 DMIBC initialization

To define the operational characteristics of a DMIBC, the physical properties and feed rates of the incoming particles are specified. The physical properties of an incoming particle are identified through its solids phase. As previously stated, the solids phase is associated with the diameter, D_m , and material density, ρ_{sm} , of a particle. Note, particles belonging to the solids phase indexed by m are identified by a subscript m and are referred to as ‘*solids phase m* ’ particles. The feed rate for each solids phase is given by a volumetric flow rate and bulk density, $\dot{V}_m$ and ρ_{bm} , respectively. Here ρ_{bm} is the

product of the material density and the volume fraction of the solids phase m particles for the feed, ε_{sm} .

Next, the flow properties for each solids phase are discretized. This is done by converting the solids phase m volumetric flow rate into an equivalent number of solids phase m particles entering the system per unit time, $N_{m,t}$. The total number of incoming particles per unit time, N_t , is given by summing $N_{m,t}$ over all solids phases.

$$N_{m,t} = \frac{\dot{V}_m}{\frac{\pi}{6} D_m^3} \quad \text{and} \quad N_t = \sum_m N_{m,t} \quad (2-1)$$

The discrete feed rate values, $N_{m,t}$ and N_t are used to establish the distribution of incoming particles. The distribution is stored in an array where each element contains the index of a single solids phase (see Figure 2-2). The number of elements that contain the index for solids phase m is proportional to the ratio $N_{m,t}/N_t$. When a particle is seeded, a random element of the distribution array is selected and the properties corresponding to the associated index are assigned to the new particle. By assigning solids phase values in this manner, the local distribution of incoming particles remains random while the globally set distribution is preserved.

Figure 2-2: Example distribution array with ten elements, three mass solids phase indices (i, j, k) with the respective distribution (20%, 30%, 50%). The fifth array element is randomly selected, leading to the incoming particle being assigned the properties associated with solids phase- j .

The discrete feed rate is adjusted to the solids time step, Δt_s , by determining the placement frequency of particles, F_p , shown in Equation (2-2). If F_p is equal to one, one or more particles is placed every solids time step. If the value is greater than one, F_p represents the number of solids time steps that transpire between the placement of individual particles.

$$F_p = \left\lfloor \frac{1}{N_t \Delta t_s} \right\rfloor \quad (2-2)$$

In Equation (2-2), $\lfloor \cdot \rfloor$, is the standard floor function that returns the integer portion of the provided value. The truncation results in the actual feed rate of solids differing slightly from the user provided parameters. This is an unavoidable consequence of translating a continuous description of the feed rate into a discrete representation.

Once the placement frequency is known, an initial velocity for each incoming solids phase, v_m^0 , is determined, shown by Equation (2-3). The feed rate and solids properties are combined with the cross-section inlet area, A_{BC} , to calculate the corresponding initial velocities for each solids phase.

$$v_m^0 = \frac{\dot{V}_m}{\frac{\rho_{bm}}{\rho_{sm}} A_{BC}} \quad (2-3)$$

The solids phase m velocities are used to determine a uniform inlet velocity that is applied to all solids phases. This prevents the generation of particle overlaps within the staging area. Without this condition, an overlap might arise due to any velocity differences. This event is illustrated in Figure 2-3, where a fast moving particle is seeded behind a slower moving particle. As the particles move toward the domain, the fast moving particle overtakes the slower moving particle resulting in an overlap between the

two particles. Once the slow moving particle fully enters the domain, the overlap is treated as the result of a collision. A sufficiently large overlap has the potential to generate an artificial spike in the total kinetic energy of the system, adversely affecting the integrity of the model. The scenario is avoided by imposing a uniform inlet velocity.

Figure 2-3: Motivation for a uniform inlet velocity. A slow moving particle is seeded behind a fast moving particle generating an artificial overlap.

The uniform inlet velocity is selected to minimize the error between user-provided and calculated bulk density values. This is accomplished through a simple iterative procedure described below.

To begin the iterative selection process for the uniform inlet velocity, the minimum and maximum phase- m velocities specified by Equation (2-3), $\min_m v_m^0$ and $\max_m v_m^0$, are used to generate $(s + 1)$ test velocity values, v_{test}^i . The calculation of the test velocities is shown in Equation (2-4). Here, s is a parameter with integer value, like 100, that influences the number of iterations.

$$v_{test}^i \in \left\{ \min_m v_m^0 + i * \frac{\max_m v_m^0 - \min_m v_m^0}{s} \mid i \in \{0, 1, \dots, s\} \right\} \quad (2-4)$$

For a given test velocity, a corresponding test bulk density is computed for each solids phase, $\tilde{\rho}_{bm}(v_{test}^i)$, shown. Here, A_{BC} is the area of the inlet region.

$$\tilde{\rho}_{bm}(v_{test}^i) = \frac{\rho_{sm} \dot{V}_m}{v_{test}^i * A_{BC}} \quad (2-5)$$

At this point, the total error, $Err_{v_{test}^i}$, between the user-defined and newly computed test bulk density values is calculated. The test velocity that produces the least amount of total bulk density error is selected. This process is repeated with a new set of test velocities established around the minimizing velocity of the previous iteration, continuing until the difference between the results of two consecutive iterations is less than a specified tolerance (e.g., 10^{-4}).

$$Err_{v_{test}^i} = \sum_m |\rho_{bm} - \tilde{\rho}_{bm}(v_{test}^i)| \quad (2-6)$$

Finally, this optimized uniform inlet velocity is compared to two velocity values, explained below. The first defines a lower bound on the inlet velocity, while the second identifies the method used to seed incoming particles. These comparisons assure that the user-defined inlet specifications are successfully managed, and determine which of the two seeding algorithms, also presented below, is employed.

The lower bound on the inlet velocity is the minimum operational velocity, v_{min} . It coincides with an unmanageable situation where particles are seeded into the staging area faster than they leave. Below v_{min} a new particle may be seeded such that it overlaps with an existing particle still within the staging area. Again, if the overlap is sufficiently large, it may cause an artificial spike in the kinetic energy of the system.

To prevent particle overlap within the staging area, a sub-grid is constructed to keep particles fully separated. The number of cells in the sub-grid, N_{BC} , depends on the

dimensions of the boundary inlet, l_{BC} and w_{BC} , and the maximum particle diameter. The calculation used to determine the number of cells is shown in Equation (2-7).

$$N_{BC} = \left\lfloor \frac{l_{BC}}{D_{max}} \right\rfloor \left\lfloor \frac{w_{BC}}{D_{max}} \right\rfloor \quad (2-7)$$

where $D_{max} = \max_m D_m$

N_{BC} is equivalent to the maximum number of disks of maximum diameter, D_{max} , that can be positioned in a square packing arrangement in a rectangle of the given dimensions. The cell sizes are uniform with their dimension based upon the maximum particle diameter to ensure that every cell can accommodate all specified particle diameters. This is a necessary condition because the diameter of an incoming particle is not established until the time of placement.

Next, a minimum inlet velocity is defined from the sub-grid and feed rate properties. Recall that if the placement frequency, F_p , is equal to one, then N_{ps} particles are seeded every solids time step, and if F_p is greater than one, one particle ($N_{ps} = 1$) is seeded every F_p solids time steps. Thus, with N_{BC} locations available within the sub-grid, it follows that $\lfloor N_{BC}/N_{ps} \rfloor$ placements can occur before two particles are seeded in the same cell. Therefore, the first N_{ps} particles that are seeded must exit the sub-grid by the time the $(\lfloor N_{BC}/N_{ps} \rfloor + 1)$ placement occurs. This assures that $(N_{ps} + N_{BC} - N_{ps} \lfloor N_{BC}/N_{ps} \rfloor)$ cells are available to receive a new particle without that particle overlapping a previously seeded particle (see Figure 2-4). The minimum inlet velocity, presented in Equation (2-8), is the direct result of this requirement, establishing the lower bound on incoming particle velocity.

$$v_{min} = \frac{D_{max}}{\Delta t_s F_p \left\lceil \frac{N_{BC}}{N_{ps}} \right\rceil} \quad (2-8)$$

Figure 2-4: Illustration of the seeding process of the grid structure. In this example, the sub-grid in the staging area contains seven cells, while two particles are placed every solids time step. Therefore, the sub-grid will overfill in four solids time steps (eight particles and only seven cells) if incoming particles do not move with sufficient speed toward the domain leaving available cells for new particles.

Once the lower bound is defined, the manner in which particles are seeded into the staging area is determined. Particles are placed either in an ordered arrangement or randomly distributed throughout the staging area.

If the staging area is densely populated, randomly placing particles potentially becomes computationally expensive. Therefore random placement is reserved for instances when a square packing would occupy less than half of the staging area at any given instant. The lower bound for the velocity correlating to less than half occupancy is given by Equation (2-9).

$$v_{rand} = \frac{D_{max}}{\Delta t_s F_p \left\lceil \left\lceil \frac{N_{BC}}{2} \right\rceil / N_{ps} \right\rceil} \quad (2-9)$$

With the velocities v_{min} and v_{rand} identified, the placement method of particles is determined. If the inlet velocity is between v_{min} and v_{rand} , particles are placed in the square packing arrangement defined by the grid structure imposed on the staging area. In this instance a fill order for the grid cells is generated. (This pattern is repeated cyclically to seed additional particles.)

For velocities greater than v_{rand} the particles are seeded via a guess-and-check (random) method. First, a particle is tentatively assigned a random location within the staging area. This position is independent of the sub-grid imposed on the staging area. Then a check is conducted to test if the location causes particle overlap with inlet particles that were previously seeded. If an overlap occurs, the particle is assigned a new random location within the staging area. This process continues until the particle is placed without any overlaps.

After a particle is seeded into the staging area, the ghost cell that contains the new particle is determined (see Figure 2-1). The cells within the computational domain that border those ghost cells in the inlet area are identified. Finally, a local search is conducted that allows for particles already within the computational domain to identify incoming particles as possible contact partners.

2.2.2 DMIBC operation

During a simulation, the placement frequency is used to calculate when the next particle is seeded. During each solids time step, the current time value is compared to a placement time, t_p . If t_p is less than or equal to the current solids time, a new particle is seeded into the inlet region, and the next seeding time updated.

$$t_p = t_p + F_p \Delta t_s \quad (2-10)$$

When a new particle is seeded, a flag is set identifying it as a new particle which indicates the dismissal of any contact forces the particle is exposed to during entry. This classification is maintained only until the particle has entered the computational domain fully. As a result, entering (new) particles will push obstructing particles in the computational domain away from the inlet.

Next, physical properties are assigned to the new particle through the appointment of a solids phase index. As previously discussed, an element from the array representing the incoming particle distribution is selected randomly. That array element contains the index of a single solids phase. From this selection, the physical properties associated with that index are assigned to the incoming particle.

After the solids phase is assigned, the center location of the new particle is determined. For an inlet using an ordered placement scheme, the sub-grid cell that will contain the new particle is identified. If the dimensions of the cell are larger than the diameter of the particle, the particle is positioned randomly within the cell; the particles that have delimited the cell dimensions are placed on cell-center. For an inlet using the random placement, the sub-grid imposed on the staging area is discarded and a guess-and-check process initiated. New locations within the staging area are assigned to the particle until it is placed without overlapping another particle.

Finally, the ghost cell that contains the new particle is determined. A local search is conducted allowing particles already within the computational domain to identify incoming particles as possible contact partners.

The positions of incoming particles are monitored during each solids time step. Once a particle has fully entered the computational domain, the flag identifying the particle as new is removed. This reclassification allows the particle to react appropriately to any force that acts upon it.

2.3 DMOBC algorithm description

The DMOBC operates in conjunction with the existing DEM framework. Namely, during the simulation a check is performed on each particle to ascertain whether or not it is in contact with any walls of the domain. If a particle is found to be in contact with a wall that contains a discrete mass outlet, an additional check is initiated. If the contact occurs at a region identified with a DMOBC, then the resulting particle-wall collision forces are dismissed. This, in effect, makes the wall *invisible* to the particle, allowing it to move out of the computational domain. This is synonymous with the process that allows incoming particles to travel from the staging area into the computational domain.

The forces acting on an exiting particle are discarded once its center crosses the domain boundary. This allows particles partially carried out of the computational domain by grid-dependent forces (e.g., gas-solids drag) to continue exiting with a constant velocity once these forces are no longer calculable.

A check is conducted at the end of each solids time step to identify particles that have fully exited the computational domain. Once a particle is completely outside the domain, a logical flag indicating the existence of the particle is removed, and the array positions associated with that particle are cleared. The vacated array positions are populated by information for incoming particles *as-needed*. By reusing the array positions, the overall amount of system resources needed during a simulation are reduced.

2.4 Implementation

The discrete mass boundary conditions were implemented into the DEM of the open-source multiphase flow software MFIX. This required the modification and creation of several subroutines. Overviews of the new subroutines are listed in Table 2-1 with their complete code included in Appendix C. Modifications to existing routines mainly consisted of logical checks associated with call statements to the new routines. A call-tree showing the invocation of the initialization routines is shown in Figure 2-5, and a call-tree showing the invocation of the operation routines is shown in Figure 2-6.

Table 2-1: A list of the subroutines comprising the discrete mass boundary conditions with brief description of their use.

Subroutine <i>file name</i>	Description
CHECK_DES_BC <i>check_des_bc.f</i>	Check the data provided for the DES mass inflow boundary condition and flag errors if the data is improper. Also, this module is used to convert the provided information into the format necessary for the dependent subroutines to function properly.
ALLOCATE_DES_MIO <i>des_allocate_arrays.f</i>	Allocate the arrays associated with the mass inflow and outflow boundary conditions.
CHECK_DES_MIO_LOCATION <i>check_des_bc.f</i>	Verify that the location of the inlet or outlet is specified on the wall of the system.
DES_BC_VEL_ASSIGN <i>des_init_bc.f</i>	Calculate the uniform inlet velocity.
DES_INIT_BC <i>des_init_bc.f</i>	Driver program; calls the necessary routines to determine the operation of the DMIBC.
DES_MI_CELLS <i>des_init_bc.f</i>	Identifies the computational fluid cells that border the DMIBC.
DES_MI_CLASSIFY <i>des_init_bc.f</i>	Classifies the plane used for seeding particles.

DES_MI_LAYOUT <i>des_init_bc.f</i>	Determines if the particles are randomly or orderly placed in the staging area.
DES_MIO_PERIODIC <i>des_init_bc.f</i>	Verifies that an inlet or outlet has not been placed on a periodic wall and that any inlet or outlet will not interfere with any periodic walls.
DES_MO_CLASSIFY <i>des_init_bc.f</i>	Classifies the plane that the outlet uses.
DES_MASS_INLET <i>des_mass_inlet.f</i>	Determines the physical properties of an incoming particle.
DES_NEW_PARTICLE_TEST <i>des_mass_inlet.f</i>	Tests to see if a randomly seeded particle is placed overlapping an existing particle.
DES_PLACE_NEW_PARTICLE <i>des_mass_inlet.f</i>	Seeds a new particle in the identified location.
DES_BC <i>des_bc_mod.f</i>	Global data storage for common boundary condition variables.
DES_CHECK_PARTICLE <i>des_check_particle.f</i>	Checks to see if an entering/exiting particle has entered/left the computational domain fully.
DES_MASS_OUTLET <i>cfwallcontact.f</i>	Checks to see if a particle in the system is interacting with a boundary region specified with a mass outlet.

Figure 2-5: Call graph of main MFX source code to initialization routines for the discrete particle model. Dashed lines indicate new calls and subroutines implemented for the discrete mass boundary conditions.

Figure 2-6: Call graph of MFX discrete particle model routines. Dashed lines indicate new calls and subroutines implemented for the discrete mass boundary conditions.

A flow chart illustrating the overall DEM algorithm implemented in MFX is presented in Figure 2-7. The additions to the algorithm including the effects of the discrete mass boundary conditions are indicated by dashed lines. If a simulation is conducted without a discrete mass boundary condition, these modifications are omitted, resulting in the original code structure.

Figure 2-7: Flow chart illustrating the locations within MFIx-DEM where modifications have been made to include discrete mass boundary condition routines.

2.5 Examples

Provided below are two examples illustrating different applications of the DMIBC. The first example, presented in Section 2.5.1, illustrates a 2D packed bed (solids

only, no gas phase) with a discrete mass inlet supplying new particles through the bottom of the bed. The second example, presented in Section 2.5.2, shows a 2D gas-solids system with an inlet gas jet coupled with a discrete mass inlet feeding particles into the bottom of the system. Both examples initially contain 500 particles comprised of five mass phases with a percent distribution for each phase of 15%, 20%, 30%, 20%, and 15%. Table 2-2 lists the physical and operating parameters of the DMIBC used in both simulations.

Table 2-2: Particle and feed properties of the examples outlined in Sections 2.5.1 and 2.5.2

Phase Index	D_m (cm)	ρ_{sm} (g/cm ³)	$\dot{V}_m$ (cm ³ /sec)	ρ_{bm} (g/cm ³)	Corresponding Distribution
1	0.100	1.75	0.00785	0.0125	0.15
2	0.125	1.85	0.02045	0.0325	0.20
3	0.150	1.95	0.05301	0.0950	0.30
4	0.175	2.05	0.05612	0.1000	0.20
5	0.200	2.15	0.06283	0.1500	0.15

2.5.1 Solids injected into a packed bed

In this first example, particles are fed into the bottom of a static particle bed operating in a vacuum (i.e., particles in the bed have zero velocity and no gas phase is present). The feed rate, N_t , is approximately 100 particles per second. The *incoming particle distribution* (the distribution of incoming particles by solids mass phase) is the same as the initial distribution of particles in the system (i.e., the percent of incoming particles in solids phases 1, 2, 3, 4, and 5 are 15%, 20%, 30%, 20%, and 15%, respectively). As previously stated, this is a global or *target* distribution for the incoming particles and is skewed on the placement frequency time scale. The computational domain is 3cm wide by 20cm tall.

Snapshots of the particle configuration within the system are shown in Figure 2-8, with only the lower 8cm of the domain displayed. For identification purposes, new particles are shaded darker than the particles initially in the system. This series of images demonstrates that incoming particles push particles already in the system away from the inlet region as they enter the computational domain.

Figure 2-8: Time series (in seconds) of particle flow for a 2D example illustrating a DMIBC injecting into a packed bed.

Figure 2-9 shows the total incoming particle distributions at three times during the simulation. The user-specified distribution of incoming particles (i.e., 15%, 20%, 30%, 20%, 15%) is shown to the right of the calculated values. This shows that the percent distribution for each solids phase is approximately maintained throughout the simulation.

Furthermore, the distribution of the particles within the system approaches the desired distribution specified by the user as the simulation progresses through time.

Figure 2-9: Cumulative incoming particle distributions at times 0.5, 3.0, and 5.0 seconds during the simulation of a DMIBC into a packed particle bed.

2.5.2 Solids injection coupled with a gas jet

This second example shows a discrete mass inlet coupled with a gas inflow boundary condition. In this simulation, the computational domain is 3cm wide and 50cm tall. A 1cm gas jet is centered on the bottom of the domain with a velocity of 1200cm/sec. A pressure outlet for the gas is specified along the top of the domain.

The simulation starts with an initial set of 500 particles in a packed bed arrangement. Initially, the velocities of the gas phase and particles are zero. During the first 3 seconds (not shown), a pseudo-steady-state is established between the gas flow and the initial particles, a time during which no particles are fed into the system. After this initial transient period, particles are fed into the system at a rate of 100 particles per second. As in the first example, the target incoming particle distribution for solids phases 1, 2, 3, 4, and 5 is 15%, 20%, 30%, 20%, and 15%, respectively (refer to Table 2-2).

Snapshots of the particle configuration within the system are shown in Figure 2-10, with only the lower 8cm displayed. Again, to distinguish new particles from initial particles, the new particles are shaded darker. Here, new particles are seen entering the computational domain and mixing with particles already in the system. This demonstrates that a DMIBC can be coupled with a continuum gas boundary condition without adversely affecting qualitative flow physics, and thereby adding new physical modeling possibilities.

Figure 2-10: Time series (in seconds) of particle flow for a 2D example illustrating a DMIBC with a gas jet.

The distribution of incoming particles (not shown) closely matches the results from the first example. This is expected since both inlets are defined by the same flow properties.

2.6 Conclusions

The current MFIX-DEM code was modified to include DMIBC and DMOBC. This allows models of more dynamic gas-solids systems by assigning user defined boundary conditions to the computational domain. The new algorithmic features have potential for use in simulations where particles enter as feedstock, like coal in a gasification model, or systems where particles are recycled, like in a circulating fluidized bed model.

Chapter 3: Particle heat transfer

Particle-particle and particle-gas heat transfer in gas-solids systems occur in the forms of conduction, convection, and radiation. The goal of this investigation is to define a mathematical model for each type of heat transfer and successfully implement the selected models into MFIX-DEM, an existing CFD-DEM.

This chapter begins by briefly defining the three modes of heat transfer and introducing the internal energy equation for a single, isothermal particle in Section 3.1. An examination into the assumption of isothermal particles is included. In the subsequent sections, an analysis of contact conduction (Section 3.2), particle-fluid-particle conduction (Section 3.3), particle-gas convection (Section 3.4), and particle-environment radiation (Section 3.5) are presented. Each investigation includes (1) a survey of models proposed in the literature, and (2) a discussion detailing modifications made to the selected model. Finally, the algorithmic implementation and verification of the selected heat transfer models are given in Sections 3.6 and 3.7.

3.1 Foundations for particle heat transfer

In this section the physical mechanisms of conduction, convection, and radiation, including a characterization of their contribution to particle heat transfer in gas-solids systems are presented briefly. Additional details concerning the fundamentals of heat transfer are found in reference [47]. The assumption of isothermal particles employed in this work is then examined. Finally, the internal energy equation of a single, isothermal particle is introduced.

3.1.1 Modes of heat transfer

Conduction is the mode of heat transfer responsible for distributing thermal energy throughout matter due to a temperature gradient. Two forms of conduction are considered in this work. *Contact conduction* occurs when two particles at different temperatures touch. As illustrated in Figure 3-1-(a), thermal energy passes from the hot particle to the cold particle through the contact area. *Particle-fluid-particle conduction* arises when two particles are in close proximity to one another. First, thermal energy is transferred from the hot particle to the intermediate gas, and then passed from the gas to the cold particle. This procedure is demonstrated in Figure 3-1-(b). Additional details concerning contact conduction and particle-fluid-particle conduction are provided in sections 3.2 and 3.3, respectively.

Figure 3-1: Illustration of conduction between particles. (a) *Contact conduction*: thermal energy is transferred from a hot particle to a cold particle through their shared contact area. (b) *Particle-fluid-particle conduction*: thermal energy is transferred from a hot particle to the stagnant gas separating its surface from the cold particle. The thermal energy is then transferred from the stagnant gas to the cold particle.

Convection in this work is defined as the transfer of thermal energy from a surface to a moving fluid due to the presence of a temperature gradient. As illustrated in Figure 3-2, convection may transfer thermal energy away from the surface of a hot particle by a cold gas, or transfer thermal energy to the surface of a cold particle by a hot gas. Additional details about convection are provided in Section 3.4.

Figure 3-2: Illustration of particle-gas convection. Thermal energy is exchanged between the surface of the particle and the moving fluid.

Radiation is the mode of heat transfer that exchanges thermal energy between two objects through the absorbing, reflecting, refracting, diffracting, and transmitting of electromagnetic waves. An illustration of radiative heat transfer is shown in Figure 3-3, where thermal energy is transmitted from a hot particle to a cold particle. A portion of the energy is absorbed by the cold particle, while some of the energy is reflected away. Additional details regarding radiation are provided in Section 3.5.

Figure 3-3: Illustration of particle-environment radiative heat transfer. Electromagnetic waves transmitted by a hot particle are absorbed and reflected by the cold particle.

3.1.2 Assumption of isothermal particles

In this work particles are assumed isothermal (i.e., no thermal gradient exists within a single particle). This assumption is examined by analyzing the conduction of thermal energy through a homogeneous, spherical particle without internal heat generation.

The governing equations for a homogeneous, spherical particle with no internal heat generation are given by Equation set (3-1) [29]. The first boundary condition asserts that the temperature distribution is continuous at the center of a particle. The second boundary condition specifies that the heat loss at the surface of a particle is equivalent to the heat transfer to the surrounding gas via convection. The initial condition assigns a temperature distribution to the particle at time, $t = 0$.

$$\rho_p C_{pp} \frac{\partial T_p}{\partial t} = \frac{1}{R_p^2} \frac{\partial}{\partial r} \left(\kappa_p R_p^2 \frac{\partial T_p}{\partial r} \right) + \frac{1}{R_p^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\kappa_p \sin \theta \frac{\partial T_p}{\partial \theta} \right) + \frac{1}{R_p^2 \sin^2 \theta} \frac{\partial}{\partial \phi} \left(\kappa_p \frac{\partial T_p}{\partial \phi} \right)$$

$$\text{with } \begin{cases} \frac{\partial T_p}{\partial r} = 0 & \text{at } r = 0 \\ \frac{\partial T_p}{\partial r} = \gamma_{cp} (T_g - T_p) & \text{at } r = r_p \\ T_p = T_{p0}(r, \theta, \phi) & \text{for } t = 0 \end{cases} \quad (3-1)$$

In Equation set (3-1), T_p , R_p , ρ_p , C_{pp} , and κ_p are a particle's temperature, radius, density, specific heat, and thermal conductivity, respectively. γ_{cp} is the convective heat transfer coefficient between a particle and gas and T_g is the average temperature of the gas surrounding a particle. By assuming that thermal conductivity is constant and that the heat transfer is radially symmetric, Equation set (3-1) is transformed through a change of variables into the dimensionless form shown in Equation set (3-2).

$$\frac{\partial \Theta}{\partial \text{Fo}_p} = \frac{1}{\eta} \frac{\partial^2}{\partial \eta^2} (\eta \Theta) \quad \text{with} \quad \begin{cases} \frac{\partial \Theta}{\partial \eta} = 0 & \text{at } \eta = 0 \\ \frac{\partial \Theta}{\partial \eta} + \Theta \text{Bi} = 0 & \text{at } \eta = 1 \\ \Theta = \Theta_0(\eta) & \text{for } \text{Fo}_p = 0 \end{cases} \quad (3-2)$$

$$\text{where } \eta = \frac{R}{R_p}, \quad \text{and } \Theta = \frac{T_p - T_g}{T_{p,ref} - T_g}.$$

$$\text{Fo}_p = \frac{\kappa_p t}{\rho_p C_{pp} R_p^2} \quad (3-3)$$

$$\text{Bi} = \frac{\gamma_{cp}}{\kappa_p / R_p} \quad (3-4)$$

In Equation set (3-2), η is the non-dimensionalized radial position in a particle of radius R_p and Θ is the non-dimensionalized temperature based on the gas temperature and some reference temperature $T_{p,ref}$. Bi is the Biot number and Fo_p is the Fourier number, both dimensionless parameters associated with a particle. The Fourier number, defined in Equation (3-3), relates the *rate* of conduction through a particle to the *rate* of heat storage within a particle, whereas the Biot number, defined in Equation (3-4), relates the convective heat transfer coefficient to the thermal conductivity within a particle. Thus, a small Biot number indicates that heat is redistributed throughout a particle faster than it is transferred from its surface via convection. As a result, a particle's core and surface temperatures are approximately the same (i.e., the particle is nearly-isothermal). In contrast, a large Biot number indicates that heat transfer via convection occurs faster than heat is redistributed inside a particle. Therefore, a particle may have different temperatures at its surface and core. These two cases are illustrated in Figure 3-4.

Figure 3-4: Illustration of Biot number classification on a particle's temperature. Arrows on the surface of the particles indicate the rate of convective heat transfer, while the arrows inside the particle represent the rate of conductive heat transfer. (a) For small Biot numbers, a particle's temperature is nearly-isothermal because the redistribution of thermal energy within a particle occurs at a faster rate than convective heat transfer. (b) When the Biot number is large, a temperature gradient may exist within a particle because the redistribution of thermal energy inside a particle is slower than the rate of convective heat transfer.

By inspection, note that the solution of the non-dimensionalized equation set is obtained through separation of variables. This leads to a Fourier series type solution, shown as Equation (3-5). Here A_n are the Fourier coefficients and λ_n the eigenvalues of the solution. Additional details related to obtaining this solution are presented in Mills [47] and Yovanovich [48].

$$\Theta = \sum_{n=1}^{\infty} A_n e^{-\lambda_n^2 \text{Fo}_p} \frac{\sin(\lambda_n \eta)}{\lambda_n \eta} \quad (3-5)$$

$$\text{where } A_n = \frac{2\text{Bi}(\lambda_n^2 + (\text{Bi} - 1)^2)}{\lambda_n^2 + \text{Bi}^2 - \text{Bi}} (-1)^{n+1} \quad \text{and} \quad \lambda_n \cos \lambda_n = (1 - \text{Bi}) \sin \lambda_n$$

Yovanovich [48] states that as the Biot number approaches zero, the first eigenvalue of the solution trends toward zero along $\sqrt{3\text{Bi}}$ as the higher order eigenvalues approach nonzero values. This observation leads to the conclusion that the first term of the series solution is dominant for small Biot numbers. Using this assumption, one can show that when Biot number is less than 0.1, a condition typically satisfied for particles in a gas-solids flow [29], the difference between the center and surface temperatures of a

particle is less than a 5% [47]. This small temperature difference across a particle in concert with the added computational complexity required to resolve the temperature within a particle leads to the general assumption that particles are isothermal in gas-solids flows. Additional details concerning this assumption are found in references [29,47]. The following section introduces the internal energy equation for a single, isothermal particle.

3.1.3 Particle internal energy equation

The internal energy for a single, isothermal particle indexed by (i) is shown in Equation (3-6) [30]. Here, m , C_{pp} , and T_p are the particle's mass, specific heat, and temperature, respectively. $\dot{Q}_{pp}^{(i)}$ is the total rate of heat transfer resulting from contact conduction, $\dot{Q}_{pfp}^{(i)}$ is the total rate of heat transfer due to particle-fluid-particle conduction, $\dot{Q}_{pg}^{(i)}$ is the rate of heat transfer between the gas and particle via convection, and $\dot{Q}_{rad}^{(i)}$ is the rate of radiative heat transfer between particle (i) and its environment. The heat of reaction supplied to the solids phase and enthalpy transfer due to mass transfer, ΔH_{rs} , are governed by the chemical reactions, if any, that the particle is undergoing.

$$m^{(i)} C_{pp}^{(i)} \frac{dT_p^{(i)}}{dt} = \dot{Q}_{pp}^{(i)} + \dot{Q}_{pfp}^{(i)} + \dot{Q}_{pg}^{(i)} + \dot{Q}_{rad}^{(i)} - \Delta H_{rs} \quad (3-6)$$

Formal definitions (mathematical models) for $\dot{Q}_{pp}$, $\dot{Q}_{pfp}$, $\dot{Q}_{pg}$, and $\dot{Q}_{rad}$ are provided in Sections 3.2 - 3.5. Further discussion of ΔH_{rs} is reserved for Chapter 4 where it is presented in the context of a mathematical interface for managing chemical reactions.

3.2 Contact conduction

Typically, heat transfer as a result of particle-particle and particle-wall contact is assumed negligible in gas-solids systems [29]. This is attributed to (1) a small contact area, and (2) the short contact duration between colliding particles [49]. However, the

contribution from contact conduction is expected to increase for highly conductive particles, as well as particles engaged in enduring contact [29,49,50]. Since a goal of this work is to construct a comprehensive heat transfer model for the CFD-DEM, contact conduction is included for completeness. The limited nature of contact conductance with respect to the overall heat transfer in a gas-solids system is further addressed in the model selection and implementation discussions.

3.2.1 Survey of particle-particle contact conduction models

This section continues by surveying several contact conduction models from the literature [49,51,52] along with various considerations that are needed to implement each model in the selected CFD-DEM framework (i.e., MFIX-DEM). Batchelor and O'Brien's [52] model is selected as the basis for the default contact conduction model developed for this work. Modifications to Batchelor and O'Brien's [52] model as employed in this work are detailed in Section 3.2.2.

3.2.1.1 Sun and Chen [49] (1988)

The contact conduction model developed by Sun and Chen [49] is based on *Hertzian theory* which relates the size of the contact area between two particles to the particles' material properties [53]. Using Hertzian theory as the basis for several assumptions, the authors hypothesize that (1) the curvatures of the particles' surfaces are negligible over the contact area, and (2) temperature changes in the particles are confined to a small region around the contact area. Both assumptions are illustrated in Figure 3-5, and lead the authors to conclude that heat transfer between two contacting particles parallels heat transfer between two *semi-infinite media*.

Figure 3-5: The elastic collision model employed by Sun and Chen [49] leads to the assumption that the shared contact area is flat.

Sun and Chen [49] further assume that (3) the thermal resistance across the contact area between two particles is negligible, and (4) the particles' surfaces are insulated outside their contact area. These assumptions are used by the authors to conclude that heat transfer is governed by two axially symmetric heat conduction equations with appropriate boundary and initial conditions. The authors make the further simplifications that (5) the physical properties of the particles are constant, (6) heat transfer is one-dimensional, occurring perpendicular to the contact area between two particles only, and (7) the Fourier numbers, defined by Equation (3-7) and based on the total contact time and maximum contact radius, are small compared to unity. Recall, a small Fourier number represents the case where the *rate* of heat conduction is small compared to the *rate* of thermal energy storage. The total contact time and maximum contact radius follow from Hertzian theory and are defined in Equations (3-8) and (3-9), respectively.

$$= \text{Fo}^{(i)'} \left(\frac{\kappa_p^{(i)}}{\rho_p^{(i)} c_{pp}^{(i)}} \cdot \frac{t_c^{(i,j)}}{(R_c^{(i,j)})^2} \right) \quad (3-7)$$

$$R_c^{(i,j)} = \left(\frac{5m^* R^{*2}}{4E^*} \right)^{1/5} \left\| \mathbf{V}_n^{(i,j)} \right\|_2^{2/5} \quad (3-8)$$

$$t_c^{(i,j)} = 2.94 \left(\frac{5m^*}{4E^*} \right)^{2/5} \left(R^* \left\| \mathbf{V}_n^{(i,j)} \right\|_2 \right)^{-1/5} \quad (3-9)$$

In these equations, $\left\| \mathbf{V}_n^{(i,j)} \right\|_2$ is the Euclidean norm (also known as the L2 norm or distance norm) of the normal impact velocity between the particles, and as before, T_p , ρ_p , C_{pp} , and κ_p are the temperature, density, specific heat, and thermal conductivity of the indexed particles. R^* and m^* are the effective radius and mass of the particles defined by Equations (3-10) and (3-11), respectively. E^* is the effective Young's modulus, and is defined by Equation (3-12), where E and ν are the Young's modulus and Poisson's ratio for the indexed particles. Young's modulus, also referred to as the *modulus of elasticity*, and Poisson's ratio are material properties of the particle.

$$R^* = \frac{R_p^{(i)} R_p^{(j)}}{R_p^{(i)} + R_p^{(j)}} \quad (3-10)$$

$$m^* = \frac{m^{(i)} m^{(j)}}{m^{(i)} + m^{(j)}} \quad (3-11)$$

$$E^* = \frac{4}{3} \left(\frac{1 - (\nu^{(i)})^2}{E^{(i)}} + \frac{1 - (\nu^{(j)})^2}{E^{(j)}} \right)^{-1} \quad (3-12)$$

Sun and Chen [49] use the assumptions outlined above to derive an analytical solution for the heat flux across the *interface* (contact area) of two touching particles. A solution for the total energy exchanged per impact for Fourier numbers approaching zero, shown as Equation (3-13), is obtained by integrating over the contact area and contact

duration. Here, c is a correction factor introduced by the authors to adjust for the assumption that heat transfer only occurs across paths perpendicular to the contact surface. Limited values for the correction factor are provided *graphically* by the authors, however a value is attainable by solving the conduction equations for contact spheres numerically.

$$\dot{Q}_{pp}^{(i,j)} = c \frac{0.87\pi \left(R_c^{(i,j)}\right)^2 \sqrt{t_c^{(i,j)}}}{\left(\rho_p^{(i)} C_{pp}^{(i)} \kappa_p^{(i)}\right)^{-1/2} + \left(\rho_p^{(j)} C_{pp}^{(j)} \kappa_p^{(j)}\right)^{-1/2}} \left(T_p^{(j)} - T_p^{(i)}\right) \quad (3-13)$$

Zhou, Yu, and Horio [54] show that the semi-infinite media assumption employed by Sun and Chen [49] over-predicts heat transfer when the Fourier number is large (e.g., heat transfer between the particle, and in turn, temperature changes in the particles are not confined to the small region around the contact area). By solving a finite element simulation of heat transfer during a particle-particle collision, the authors develop an analytic expression for the correction factor, shown as Equation (3-14). Zhou, Yu, and Horio [54] assert that their correction factor in conjunction with Sun and Chen's model [49] better approximates heat transfer between smooth, spherical particles with Fourier number as large as 10. The correction is formulated for the specific case where the thermal conductivity of the colliding particles are equal, and the authors suggest conducting a finite element simulation to reformulate Equation (3-14) varying particle thermal conductivities (i.e., $\kappa^{(i)}/\kappa^{(j)} \neq 1$) for best results.

$$c' = \frac{0.43 \left(\sqrt{c_2^2 - 4c_1(c_3 - \text{Fo}')} - c_2 \right)}{c_1}$$

$$\begin{aligned} c_1 &= -2.300\beta^2 + 8.909\beta - 4.235 \\ \text{where } c_2 &= 8.169\beta^2 - 33.770\beta + 24.885 \quad \text{and} \quad \beta = \frac{\rho_p^{(i)} C_{pp}^{(i)}}{\rho_p^{(j)} C_{pp}^{(j)}} \\ c_3 &= -5.758\beta^2 + 24.464\beta - 20.511 \end{aligned} \quad (3-14)$$

The original model proposed by Sun and Chen [49] is found in several CFD-DEM codes [17,18,55], as well as Zhou, Yu, and Horio's [54] correction factor [19,20]. One limitation of Sun and Chen's [49] model is the level of computational resources needed to evaluate Equations (3-7), (3-8), (3-9), (3-10), (3-11), (3-12), (3-13), and possibly (3-14) for *each occurrence* of particle-particle conduction. This amount of computational expense is considered excessive given that contact conduction is not anticipated to contribute substantially to the overall heat transfer in gas-solids systems [29,49,50]. Another limitation of Sun and Chen's [49] model is its dependence on a correction factor. The authors provide two graphs for approximating the correction. Numerical experiments, like that employed by Zhou, Yu, and Horio [54], produce specific values or analytic expressions for the correction factor, but require substantial effort to obtain. Due to its computational expense and dependence on a correction factor, this model was not selected for this work.

3.2.1.2 Shimizu [51] (2006)

Another model proposed for contact conduction is employed in the software PFC2D/3D [56,57], and is presented in the work of Shimizu [51]. In this approach, illustrated in Figure 3-6, thermal energy is exchanged between two particles through a *thermal pipe*. The rate of heat transfer between particles (*i*) and (*j*) across the thermal pipe is given by Equation (3-15). Here, $\ell^{(i,j)}$ is the distance between the centers of the

particles and delineates the length of the thermal pipe, $A_c^{(i,j)}$ is the contact area between the two particles and defines the cross-sectional area of the pipe, and $\psi^{(i,j)}$ is the thermal resistance of the pipe.

Figure 3-6: Particle-particle conduction model employing a thermal pipe connecting the centers of two particles. Implemented in PFC2D/3D [56,57] and presented by Shimizu [51].

$$\dot{Q}_{pp}^{(i,j)} = \frac{(T_p^{(j)} - T_p^{(i)})}{\psi^{(i,j)} l^{(i,j)}} \quad (3-15)$$

The complexity of this model arises from the need to obtain a value for the resistance of the thermal pipes, $\psi^{(i,j)}$. First, the author analyzes Fourier's Law of Conduction, shown as Equation (3-16), for a *particle assembly*. The term particle assembly defines a collection of particles in a predefined control volume (CV). Here, $\kappa_{\mathfrak{L}}$ and $T_{\mathfrak{L}}$ are the thermal conductivity and temperature of the particle assembly, respectively. $T_{\mathfrak{L}}$ is defined as the arithmetic average particle temperature in the assembly. The definition of $\kappa_{\mathfrak{L}}$ is more complex as discussed below. In this work the symbol $\mathfrak{L}$ is used to denote the particle assembly containing the (i,j) particle pair as illustrated in Figure 3-7.

$$\mathbf{q}_{\mathfrak{L}} = -\kappa_{\mathfrak{L}} \frac{\partial T_{\mathfrak{L}}}{\partial x_i} \quad (3-16)$$

Figure 3-7: Illustration of a particle assembly as defined by Shimizu [51] with interconnected thermal pipes.

Shimizu [51] then equates the heat flux of the assembly, $\mathbf{q}_{\mathfrak{L}}$, to the volume averaged heat flux across all the thermal pipes within the assembly, shown as Equation (3-17). In this equation, $\mathcal{V}_{CV}$ is the volume of the CV, and $N_{\mathfrak{L},tp}$ is number of thermal pipes in particle assembly $\mathfrak{L}$. For the thermal pipe indexed by (m) , ℓ , ∇T , and ψ are its length, temperature gradient, and thermal resistance, respectively. ξ is the unit vector directed along the thermal pipe indexed by (m) .

$$\mathbf{q}_{\mathfrak{L}} = -\frac{1}{\mathcal{V}_{CV}} \sum_{m=1}^{N_{\mathfrak{L},tp}} \frac{\ell^{(m)} \xi^{(m)} \cdot \xi^{(m)T}}{\psi^{(m)}} \nabla T^{(m)} \quad (3-17)$$

Shimizu [51] goes on to replace the individual thermal pipe (microscopic) temperature gradients, $\nabla T^{(m)}$, with the assembly (macroscopic) temperature gradient, $\nabla T_{\mathfrak{L}}$. By comparing the result with Equation (3-16), Equation (3-18) is established as the definition for the thermal conductivity of the assembly.

$$\mathbf{\kappa}_{\mathfrak{L}} = \frac{1}{\mathcal{V}_{CV}} \sum_{m=1}^{N_{\mathfrak{L},tp}} \frac{\ell^{(m)} \xi^{(m)} \cdot \xi^{(m)T}}{\psi^{(m)}} \quad (3-18)$$

Shimizu [51] then assumes that (1) heat transfer in the assembly is *isotropic* (directionally invariant) and (2) the thermal resistance is uniform for all thermal pipes in the assembly (i.e., $\psi_{\mathcal{Q}} = \psi^{(m)} \forall m \in \mathcal{Q}$). Thus, the thermal conductivity of the assembly is defined as the mean value of the diagonal elements of the thermal conductivity tensor, $\kappa_{\mathcal{Q}}$, as shown in Equation (3-19). Here, the three in the denominator arises from the spatial dimension of the given problem (in this case, 3-D).

$$\bar{\kappa}_{\mathcal{Q}} = \frac{1}{3\mathcal{V}_{CV}\psi_{\mathcal{Q}}} \sum_{m=1}^{N_{\mathcal{Q},tp}} \ell^{(m)} \quad (3-19)$$

Equation (3-19) is then rearranged to develop an expression for the thermal resistance of the assembly, as shown in Equation (3-20). Once a value for the thermal resistance of the assembly is attained, it is used to represent the thermal resistance of each thermal pipe ($\psi^{(i,j)} = \psi_{\mathcal{Q}}$). That is, it substituted back into Equation (3-15) to evaluate the rate of heat transfer between the two contacting particles.

$$\psi_{\mathcal{Q}} = \frac{1}{3\bar{\kappa}_{\mathcal{Q}}\mathcal{V}_{\mathcal{Q}}} \sum_{m=1}^{N_{\mathcal{Q},tp}} \ell^{(m)} \quad (3-20)$$

Careful examination reveals that Shimizu's [51] published equations (i.e., Equation (3-20)) are underdetermined. Specifically, a secondary expression for the thermal conductivity of the particle assembly ($\bar{\kappa}_{\mathcal{Q}}$) is needed to obtain a meaningful model. The author does not explicitly state how this value is obtained, or if it is taken as some average of the particles' thermal conductivity.

This model poses several limitations, most notably, the underdetermined definition for the thermal conductivity of the particle assembly ($\bar{\kappa}_{\mathcal{Q}}$). Additionally, this

approach appears better suited for simulations where particle movement is limited. In gas-solids flows where particles are always moving, the members comprising the particle assemblies are continually changing. In turn, the thermal resistances of the assemblies require recalculation at each solids time step. Due to the ambiguity of the model and the avoidable computational expense of calculating thermal resistances, this model is dismissed in favor of a well-defined, simpler model.

3.2.1.3 Batchelor and O'Brien [52] (1977)

Batchelor and O'Brien [52] also developed a contact conduction model based on Hertzian collision theory. Unlike the model of Sun and Chen [49] which employs a maximum contact radius, Batchelor and O'Brien [52] use the instantaneous compression force (normal contact force) to calculate the contact radius, shown in Equation (3-21). R^* and E^* are the effective radius and Young's modulus previously defined in Equations (3-10) and (3-12), respectively. $\mathbf{F}_n^{(i,j)}$ is the normal force resulting from the collision/contact between two particles indexed by (i) and (j) .

$$R_c^{(i,j)} = \left(\frac{2R^*}{E^*} \left\| \mathbf{F}_n^{(i,j)} \right\|_2 \right)^{1/3} \quad (3-21)$$

By drawing a comparison between the velocity potential of an incompressible fluid through a circular hole in a plane wall, and the temperature distribution inside the particles, Batchelor and O'Brien [52] obtain an expression for the energy flux normal to the contact area of two particles. The energy flux is given by Equation (3-22), and illustrated in Figure 3-8. Integrating Equation (3-22) over the contact area gives total rate of heat transfer between the particles per unit time, shown as Equation (3-23).

$$q_c^{(i,j)} = \frac{\kappa_p (T_p^{(j)} - T_p^{(i)})}{\pi \sqrt{R_c^{(i,j)} - r^2}} \quad \text{for } r \in [0, R_c^{(i,j)}] \quad (3-22)$$

Figure 3-8: Illustration of the thermal energy flux from a hot particle to a cold particle across the contact area.

$$\dot{Q}_{pp}^{(i,j)} = 2\kappa_p R_c^{(i,j)} (T_p^{(j)} - T_p^{(i)}) \quad (3-23)$$

This model was selected as the foundation for developing a contact conduction model in this work. The selection was guided by (1) the algebraic simplicity of the model, and (2) the wide employment of this model for particle-particle conduction in CFD-DEM [58,59,19,22,60,61]. Specific modifications to Batchelor and O'Brien's [52] model are presented in the following section wherein limitations of this model are addressed. In particular, Batchelor and O'Brien's [52] model assumes that particles have the same thermal conductivity, κ_p , and employs a Hertzian collision model as a basis for calculating the contact area. Finally, assumptions needed to extend the two-particle contact conduction model to a multiple-particle contact conduction model are presented. Specifically, what assumptions need satisfied so that simultaneous instances of contact conduction for the same particle (i.e., a particle experiences contact conduction with two or more particles at the same time) are summable, resulting in an expression for the total amount of contact conduction the particle experiences.

3.2.2 Modified Batchelor and O'Brien [52] two-particle contact conduction model

A constraint of Batchelor and O'Brien's [52] contact conduction model is the assumption that both particles have the same thermal conductivity, κ_p . This prohibits the use of the model in systems where particle types, and in turn thermal conductivities of the particles, may vary. Their model is extended in this work by defining an effective thermal conductivity between two particles, shown in Equation (3-24). As defined, the smaller thermal conductivity controls the rate of heat transfer across the contact area. This is consistent with the *thermal circuit* concept put forward by Mills [47], whereby heat transfer across a composite wall is limited by the material with the highest resistance to conductive heat transfer. Likewise, Zhou, Yu, and Zulli [19] impose a similar modification to Batchelor and O'Brien's [52] model in their work.

$$\kappa_p^* = 2 \left(\frac{1}{\kappa_p^{(i)}} + \frac{1}{\kappa_p^{(j)}} \right)^{-1} \quad (3-24)$$

In Batchelor and O'Brien's [52] derivation, they employ a Hertzian collision model to determine the area of contact through which heat may flow. In this effort, their model is generalized further by using the geometric configuration of the two particles to obtain the radius of their shared contact area. This approach results in a contact area representative of the specific collision model employed by the DEM (e.g., Cundall and Strack [44], Hertz [53], etc.), and promotes greater modeling consistency throughout the CFD-DEM. Equation (3-25) defines the contact radius employed in this work. The indices k and l are used to identify the particles by diameter size, specifically $R_p^{(k)} = \max\{R_p^{(i)}, R_p^{(j)}\}$ and $R_p^{(l)} = \min\{R_p^{(i)}, R_p^{(j)}\}$; and, $\ell^{(i,j)}$ is the distance separating the

particles' centers. Formal algebraic and geometric definitions of these terms are reserved for Appendix B.

$$\tilde{R}_c^{(i,j)} = \sqrt{R_p^{(k)^2 - \left(\frac{R_p^{(k)^2} - R_p^{(l)^2} + \ell^{(i,j)^2}}{2 \ell^{(i,j)}} \right)^2}} \quad (3-25)$$

Substituting Equations (3-24) and (3-25) into Equation (3-23) results in the contact conduction model developed and implemented in this work, shown as Equation (3-26).

$$\dot{Q}_{pp}^{(i,j)} = \frac{4\kappa_p^{(i)} \kappa_p^{(j)}}{\kappa_p^{(i)} + \kappa_p^{(j)}} \sqrt{R_p^{(k)^2 - \left(\frac{R_p^{(k)^2} - R_p^{(l)^2} + \ell^{(i,j)^2}}{2 \ell^{(i,j)}} \right)^2}} (T_p^{(j)} - T_p^{(i)}) \quad (3-26)$$

This model, as well as those presented in Section 3.2.1, is derived in the context of two particle systems (i.e., contact conduction only occurs between two individual particles). The following section explains the extension of this model to situations where a particle may undergo contact conduction with several neighboring particles simultaneously.

3.2.3 Extension to multi-particle systems

The model developed for this work and those described in Section 3.2.1 are based on two particle systems. Vargas [62] states that the individual instances of contact conduction are summable under two conditions. First, the Biot numbers associated with a collision, defined in Equation (3-27), must remain small compared to unity. Physically, a small Biot number ensures that the rate of heat transfer between two particles is slow in comparison to the rate of thermal energy redistributed inside each particle. Conversely, the resistance to heat transfer inside a particle is much smaller than the resistance

between particles. Thus, all particles touching a particle will witness the same temperature for that particle. This is consistent with the argument used in this work to justify the assumption of isothermal particles (see Section 3.1.2).

$$\text{Bi}' = \frac{2\kappa_p^* \tilde{R}_c^{(i,j)} / A_p^{(i)}}{\kappa_p^* / R_p^{(i)}} = \frac{2\tilde{R}_c^{(i,j)}}{\pi R_p^{(i)}} \ll 1 \quad \text{for } j \in \mathfrak{A} \quad (3-27)$$

The second assumption, according to Vargas [62], is that a particle's temperature must change gradually so that fluctuations in temperature do not propagate beyond its immediate neighbors over one solids time step. This *quasi-steady temperature criterion* [62] is given by Equation (3-28). Here $\Delta T_p^{(i)}$ represents the temperature change of particle i over a solids time step of duration Δt_s . This is recast in Equation (3-29) to generate an upper bound on the size of the solids time step. Vargas [62] states that this bound is easily met within the framework of the CFD-DEM as it is orders of magnitude less restrictive than the bound placed on the solids time step for numerical stability of the collision model.

$$\frac{\Delta T_p^{(i)}}{T_p^{(j)} - T_p^{(i)}} = \frac{2\kappa_p^* \tilde{R}_c^{(i,j)}}{m^{(i)} C_{pp}^{(i)}} \Delta t_s \ll 1 \quad \text{for } j \in \mathfrak{A} \quad (3-28)$$

$$\Delta t_s \ll \frac{m^{(i)} C_{pp}^{(i)}}{2\kappa_p^* \tilde{R}_c^{(i,j)}} \quad \text{for } j \in \mathfrak{A} \quad (3-29)$$

This completes the discussion of contact conduction. Here, Equation (3-26) is established as the default contact conduction model ($\dot{Q}_{pp}$) for the particle internal energy equation (Equation (3-6)). The subsequent section introduces various models for particle-fluid-particle conduction ($\dot{Q}_{pfp}$) presented in the literature as well as considerations for implementing them into the framework of the CFD-DEM.

3.3 Particle-fluid-particle conduction

In addition to contact conduction, particles in close proximity to one another may also transfer energy by conducting heat through the stagnant gas separating their surfaces. Wen and Chang [63] suggest this form of conduction may contribute between 10-35% of the total heat transferred among solids in some gas-solids systems.

3.3.1 Survey of particle-fluid-particle conduction models

This section begins by surveying several particle-fluid-particle conduction models from the literature [16,63,64,65] along with various considerations that are needed to implement each model in the selected CFD-DEM framework (i.e., MFIX-DEM). Rong and Horio's [16] model is selected as the basis for the particle-fluid-particle conduction model developed in this work. Modifications to Rong and Horio's [16] model are discussed in Section 3.3.2.

3.3.1.1 Wen and Chang [63] (1967)

Wen and Chang [63] proposed a simple analytic model for heat transfer in gas-solids systems operating at low temperatures and containing two types of particles (i.e., type A and type B particles). Particles of the same type are assumed identical in physical and thermal properties as well as temperature. The authors hypothesize that heat transferred from a particle's surface primarily results from particle-gas convection and particle-fluid-particle heat transfer. Contact conduction and radiative heat transfer are assumed insignificant for their case (i.e., particulate fluidization at temperatures below 600°C). They conclude that the total flux of thermal energy across the surface of a type A particle is given by Equation (3-30). The first component on the right hand side is the

flux due to particle-gas convection, while the second component is the result of particle-fluid-particle conduction.

$$\dot{q}_A = \gamma_{cp}(T_A - T_g) + \gamma_{BA}(T_A - T_B) \quad (3-30)$$

In Equation (3-30), γ_{cp} is the convective heat transfer coefficient between the gas and a type A particle, γ_{BA} is the particle-particle heat transfer coefficient, and T_A , T_B , and T_g are the temperatures of the type A and B particles and gas, respectively. Wen and Cheng [63] determined the particle-particle heat transfer coefficient through physical experimentation.

The simplified analysis of heat transfer used to construct this model prevents it from functioning as a general particle-fluid-particle conduction model. For example, the authors hypothesize that contact conduction and radiative heat transfer are negligible, limitations not imposed in the present work. In addition, enforcing the authors' assumption that particles of the same type have the same temperature requires that each Type A particle (or Type B particle) experience the same total heat flux. Otherwise, the individual particles temperatures may diverge as the solutions to the internal energy equations for the particles (i.e., Equation (3-6)) are advanced. Finally, expressions for the particle-particle heat transfer coefficients are scarcely available and limit this model's validity to cases from which correlations are derived. As such, Wen and Chang's [63] model was not selected for this work.

3.3.1.2 Delvosalle and Vanderschuren [64] (1985)

Delvosalle and Vanderschuren [64] developed an analytic model for particle-fluid-particle conduction by considering heat transfer between two isothermal particles in a stagnant medium with negligible heat capacity. They hypothesize that for large

spherical particles of the same size, heat transfer between particles is restricted to a small region around the axis relating the particles' centers. They further assume that heat transfer paths are portions of circumferences perpendicular to the particles' surfaces, as illustrated in Figure 3-9.

Figure 3-9: Illustration depicting the heat transfer paths as defined by Delvosalle and Vanderschuren's [64]. The heat transfer paths are defined as portions of circumferences perpendicular to the surfaces of the particles.

The resulting model for the instantaneous rate of heat transfer between the particles indexed by (*i*) and (*j*) is given Equation (3-31). Here, R_p is the particle radius, s is distance between the particles' surfaces, and α is the angle delineating the region of particle-fluid-particle conduction. The quantity inside the integral represents the length of the heat transfer paths through the stagnant medium.

$$\dot{Q}_{pfp}^{(i,j)} = \pi \kappa_g R_p (T_p^{(j)} - T_p^{(i)}) \int_0^\alpha \frac{\sin^2 \theta}{2[s/R_p + (1 - |\cos \theta|)]\theta} d\theta \quad (3-31)$$

Delvosalle and Vanderschuren [64] extend this model to fluidized systems (i.e., multiple particles in the presents of a non-stagnant gas) in their definition of α . The authors assume laminar sub-layers, spherical in shape, develop around particles due to gas flow. Particle-fluid-particle conduction initiates when the sub-layer surrounding one particle intersects the sub-layer surrounding another particle. This is illustrated in Figure 3-10. The resulting definition for α is given by Equation (3-32). Here, d is the thickness

of the sub-layer and is defined by the authors as the ratio of gas phase thermal conductivity to the heat transfer coefficient of the solids phase.

Figure 3-10: Delvosalle and Vanderschuren's [64] model assumes particle-fluid-particle conduction is initiated when the laminar sub-layers surrounding two particles overlap. This configuration is used to define the parameter α in Equation (3-42).

$$\cos \alpha = \frac{R_p + s/2}{R_p + d} \quad (3-32)$$

In their model, Delvosalle and Vanderschuren [64] observed that the rate of heat transfer grows infinitely as the distance separating the particles' surfaces approach zero (i.e., $\lim_{s \rightarrow 0} Q_{pfp}^{(i,j)}$). They conclude that *perfect contact* between particles ($s = 0$) is prohibited by surface roughness, and therefore hypothesize the existence of a minimum separation distance, s_m . By imposing the minimum separation distance between the particles' surfaces, the rate of heat transfer between the particles is bounded.

Delvosalle and Vanderschuren's [64] model is limited to gas-solids systems where solids are characterized by equal sized particles (i.e., monodispersity). Furthermore, inspection of Equation (3-31) shows that this model does not extend to include particles of varying size (i.e., polydispersity). Specifically, the paths of heat transfer are not definable as portions of circumferences of circles perpendicular to the surfaces of the particles if the diameters of two neighboring particles are different. (It is a geometric impossibility.) Since gas-solids flows are not typically monodisperse [66],

selecting this approach introduces unnecessary limitations into the CFD-DEM. Although Delvosalle and Vanderschuren's [64] model is implemented in various CFD-DEM codes [59,67], it was not selected for this work in lieu of a more general approach.

3.3.1.3 Cheng, Yu, and Zulli [65] (1999)

Cheng, Yu, and Zulli [65] developed two structure-based analytic models for particle-fluid-particle conduction. Both models assume that heat transfer between two neighboring particles is restricted to the region delineated by the *double pyramid* defined by a Voronoi tessellation boundary plane, illustrated in Figure 3-11. The authors simplify the geometry of the heat transfer region by replacing the double pyramid with a *double tapered cone* that has the same volume and distance between vertices (particles' centers).

Figure 3-11: The model of Cheng, Yu, and Zulli [65] restricts particle-fluid-particle conduction to the region delineated by the double pyramid (3-D) generated by the Voronoi-boundary plane.

Cheng, Yu, and Zulli [65] employ several assumptions to construct their first model, *Model A*, including (1) the surface of the double tapered cone is isothermal, (2) conduction is negligible in the outer region of the double tapered cone, and (3) the heat transfer paths are parallel to the axis joining the particles' centers. These assumptions are illustrated in Figure 3-12. The resulting model for the rate of heat transfer between particles (*i*) and (*j*) is given as Equation (3-33).

Figure 3-12: Cheng, Yu, and Zulli's [65] Model A for particle-fluid-particle conduction assumes that the surface of the double tapered cone is isothermal, conduction is negligible in the outer region of the double tapered cone, and the heat transfer paths are parallel to the axis joining the particles' centers.

$$\dot{Q}_{pfp}^{(i,j)} = (T_p^{(j)} - T_p^{(i)}) \int_{r_s}^{r_g} \left(\frac{2\pi r}{\ell_{ir}/\kappa_p^{(i)} + \ell_{gr}/\kappa_g + \ell_{jr}/\kappa_p^{(j)}} \right) dr \quad (3-33)$$

In Equation (3-33), r_s and r_g define the fluid region for conduction. Specifically, r_s defines the inner boundary (zero if the particles are not touching and the radius of the contact area if touching) and r_g defines the outer boundary. ℓ_{ri} and ℓ_{rj} are the lengths of the heat transfer paths through the i^{th} and j^{th} particles, and ℓ_{rg} is the length of the heat transfer path through the gas, respectively. As previously indicated, T_p and κ_p are the temperatures and thermal conductivities of the indexed particles, κ_g is the thermal conductivity of the gas, and $\ell^{(i,j)}$ is distance between the particles' centers. The geometric representation of these quantities is illustrated in Figure 3-13.

Figure 3-13: Geometric representation of quantities used by Cheng, Yu, and Zulli's [65] Model A for particle-fluid-particle conduction.

To develop their second model for particle-fluid-particle conduction, *Model B*, Cheng, Yu, and Zulli [65] assume (1) each particle has an isothermal core of radius R_c , and (2) heat transfer paths radiate from the cores' surfaces. These assumptions are illustrated in Figure 3-14, and the resulting model for the rate of heat transfer between particles (i) and (j) is given as Equation (3-34).

Figure 3-14: Cheng, Yu, and Zulli's [65] *Model B* for particle-fluid-particle conduction assumes that each particle has an isothermal core and the paths of heat transfer radiate from the particles centers.

$$\dot{Q}_{pfp}^{(i,j)} = \pi (T_p^{(j)} - T_p^{(i)}) \frac{1}{b} \ln \left(\frac{a - b \cos \theta_0}{a - b \cos \theta_c} \right) \quad (3-34)$$

$$a = \frac{1}{2} \left(\frac{1}{\kappa_p^{(i)}} + \frac{1}{\kappa_p^{(j)}} \right) \left(\frac{1}{R_c} - \frac{1}{R_p} \right) + \frac{1}{\kappa_g R_p}; \quad b = \frac{1}{\kappa_g (R_p + s/2)}$$

In Equation (3-34), θ_0 and θ_c define the fluid region for conduction. Specifically, θ_c defines the inner boundary (zero if the particles are not touching and the angle delineating the contact area if touching), θ_0 defines the outer boundary, and s is distance between the particles' surfaces.

A significant drawback to Cheng, Yu, and Zulli's [65] models is their dependence on a Voronoi tessellation to determine the region of particle-fluid-particle heat transfer. Due to the continuous movement of particles in gas-solids systems, a tessellation is required at each solids time step. Such calculations are computationally expensive. Additionally, since their models were developed for packed bed simulations, extending

them to fluidized systems may result in unphysical behavior. Specifically, particles that are separated by large distances may share common Voronoi-boundaries, and in turn, have the potential to engage in particle-fluid-particle heat transfer. Additional constraints are needed to prevent this from occurring in the current model (i.e., a maximum distance at which particle-fluid-particle ceases to occur). Finally, introducing models which consider resistance to heat transfer through particles is contradictory to the assumption in the present effort that particles are isothermal (see Section 3.1.2). Although a simplified version of *Model A* is found in the CFD-DEM model of Zhou, Yu, and Zulli [19], neither *Model A* nor *Model B* is selected for this work. This is due to the computational complexity of the models and disagreement with the fundamental assumption employed in this work of isothermal particles.

3.3.1.4 Rong and Horio [16] (1999)

Rong and Horio [16] introduced a particle-fluid-particle heat transfer model similar to that of Delvosalle and Vanderschuren [64]. The authors hypothesize that (1) each particle is surrounded by a gas layer with thickness $\delta = R_p$, and (2) particle-particle heat transfer initiates when the gas layer surrounding a particle intersects with the surface of another particle. They further assume that (3) heat transfer occurs across paths parallel to the axis joining the particles' centers, and (4) a uniform gas layer, $4.0 \times 10^{-10}m$ thick, separates the particles' surfaces as they collide. These assumptions are illustrated in Figure 3-15. The resulting model is given in Equation (3-35).

Figure 3-15: Rong and Horio's [16] configuration for particle-fluid-particle conduction. In their model, each particle is surrounded by a gas layer and heat transfer occurs across paths parallel to the line connecting the centers of the particles. When particles engage in contact, the overlap region is assumed to have a uniform gas layer separating the particles' surfaces.

$$\dot{Q}_{pfp}^{(i,j)} = \kappa_g (T_p^{(j)} - T_p^{(i)}) \mathcal{A}$$

where

$$\mathcal{A} = \begin{cases} 0 & \text{for } \ell^{(i,j)} \geq 3R_p \\ \int_0^\alpha \frac{2\pi R_p \sin \theta}{\ell^{(i,j)} - 2R_p \cos \theta} d(R_p \sin \theta) & \text{for } 3R_p > \ell^{(i,j)} > 2R_p \\ \frac{\pi(R_p \sin \beta)^2}{4 \times 10^{-10}} + \int_\beta^\alpha \frac{2\pi R_p \sin \theta}{\ell^{(i,j)} - 2R_p \cos \theta} d(R_p \sin \theta) & \text{for } \ell^{(i,j)} \leq 2R_p \end{cases} \quad (3-35)$$

In Equation (3-35), α and β are the angles delineating the region of particle-fluid-particle conduction, $\ell^{(i,j)}$ is the distance between the centers of the particles, κ_g is the thermal conductivity of the gas, and R_p and T_p are the particles radius and temperature, respectively. Particles whose surfaces are separated by a distance greater than one particle radius (R_p) do not undergo particle-fluid-particle heat transfer. When the surfaces of two particles are closer than one particle radius but not touching particle-fluid-particle heat transfer occurs in the defined region. If two particles are in direct contact, then there is a uniform rate of particle-fluid-particle heat transfer across the contact area

$\left(\frac{\pi(R_p \sin \beta)^2}{4 \times 10^{-10}}\right)$ as particle-fluid-particle heat transfer occurs around the interface of the contact area.

This model was selected as the foundation for the particle-fluid-particle model developed in this work. Like the model proposed by Delvosalle and Vanderschuren [64], Rong and Horio's [16] approach is valid only for particles of equal diameter. However, unlike Delvosalle and Vanderschuren's [64] model, the model proposed by Rong and Horio [16] extends to particles of different sizes by modifying several geometric definitions. The extension is possible because Rong and Horio [16] assume that heat transfer paths are parallel to the axis joining the particles' centers as opposed to the arc structures used by Delvosalle and Vanderschuren [64]. The following section presents the extension of Rong and Horio's [16] model to include particles of different sizes.

3.3.2 Modified Rong and Horio [16] particle-fluid-particle conduction model

As previously noted, Rong and Horio's [16] model for particle-fluid-particle conduction was developed in the context of equal size particles. Extending their model to particles of different size requires a standard point of reference to develop a consistent definition for the particle-fluid-particle region. This specification is satisfied by delineating the outer region of particle-fluid-particle heat transfer by the intersection of the gas layer surrounding the larger particle with the surface of the smaller particle. This is expressed by Equation (3-36) and illustrated in Figure 3-16. Here, the indices (k) and (l) identify the particles by size, specifically $R_p^{(k)} = \max\{R_p^{(i)}, R_p^{(j)}\}$ and $R_p^{(l)} = \min\{R_p^{(i)}, R_p^{(j)}\}$, and $d^{(k)}$ is the thickness of the gas layer. $R_f^{(i,j)}$ is similar to α in Equation (3-35) in that it delineates the upper bound on the region of particle-fluid-

particle conduction. The default gas layer thickness for a particle indexed by (i) is defined as $R_p^{(i)}/5$ in the current effort. This value was suggested by Xavier and Davidson [68] in their surface-to-bed heat transfer studies using 0.1-8.0mm particles and a vertical heater.

$$R_f^{(i,j)} = \sqrt{\left(R_p^{(k)} + d^{(k)}\right)^2 - \left(\frac{\left(R_p^{(k)} + d^{(k)}\right)^2 - R_p^{(l)2} + \ell^{(i,j)2}}{2\ell^{(i,j)}}\right)^2} \quad (3-36)$$

Figure 3-16: Illustration of geometric quantities delineating the region of particle fluid heat transfer imposed in this work.

A change of variable is applied to Rong and Horio's [16] model to remove its dependency on the trigonometric functions of sine and cosine. This change was established so that standard quadrature routines are capable of managing the integral term. Finally, the additional quantity added by Rong and Horio [16] to account for heat transfer in the contact region (i.e., $\pi(R_p \sin \beta)^2/4 \times 10^{-10}$ in Equation (3-35)) is discarded in lieu of the contact conduction model defined in Section 3.2.2. The resulting model for particle-fluid-particle heat transfer is given as Equation (3-37). Here, $\tilde{R}_c^{(i,j)}$ is the contact radius of two touching particles defined in Equation (3-25) and $\ell^{(i,j)}$ is the distance separating the particles' centers.

$$\dot{Q}_{pfp}^{(i,j)} = \kappa_g (T_p^{(j)} - T_p^{(i)}) \int_{R_c}^{R_f^{(i,j)}} \frac{2\pi r}{\ell^{(i,j)} - \left((R_p^{(i)^2} - r^2)^{1/2} + (R_p^{(j)^2} - r^2)^{1/2} \right)} dr \quad (3-37)$$

where

$$R_c = \begin{cases} 0 & \text{for } \ell^{(i,j)} > 2R_p \\ \tilde{R}_c^{(i,j)} & \text{for } \ell^{(i,j)} \leq 2R_p \end{cases}$$

As illustrated in Figure 3-17, a singularity in the integral term of Equation (3-37) occurs at the interface of two touching particles. This results in an infinite rate of heat transfer between the particles. Delvosalle and Vanderschuren [64] also observed this problem and avoided *perfect contact* between the particles by requiring a minimum separation distance. In this effort, a default minimum separation distance of $4 \times 10^{-10} \text{m}$ is specified, which corresponds to the value used for surface roughness in Rong and Horio's [16] model.

Figure 3-17: A singularity arises in the modified Rong and Horio model at the interface of the contact boundary. This is corrected by prohibiting perfect contact between particles, and require a minimum separation distance of $4 \times 10^{-10} \text{m}$. Similar assumptions are employed by Delvosalle and Vanderschuren [64] and Rong and Horio [16].

This completes the section on particle-fluid-particle heat transfer. Here, Equation (3-37) is established as the default particle-fluid-particle conduction model ($\dot{Q}_{pfp}$) for the

particle internal energy equation (Equation (3-6)). The following section considers particle-gas convective heat transfer ($\dot{Q}_{pg}$) in gas-solids systems.

3.4 Particle-gas convection

Recall, convection is defined in this effort as heat transfer between a particle and the surrounding gas resulting from differences in temperature and velocity. This section introduces Newton's law of cooling for modeling convection, and briefly discusses the connection between the convective heat transfer coefficient and dimensionless Nusselt number. The Ranz and Marshall [69] correlation for the Nusselt number, selected as the default correlation in this work, is presented.

3.4.1 Background of particle-gas convection

Heat transfer between a particle and gas is assumed in this work to follow Newton's law of cooling. Newton's law of cooling, shown as Equation (3-38), hypothesizes that the rate of heat transfer between two objects is proportional their temperature difference. The constant of proportionality for convective heat transfer between a particle and gas often is given as the combination of a convective heat transfer coefficient (γ_{cp}) and the surface area of the particle (A_s). Therefore, the rate of convective heat transfer between a single particle and moving gas is given by Equation (3-39), where T_p is the particle's temperature, and T_g is the average temperature of the gas surrounding the particle.

$$\dot{Q}_{pg} \propto \Delta T \quad (3-38)$$

$$\dot{Q}_{pg} = \gamma_{cp} A_s (T_g - T_p) \quad (3-39)$$

The convective heat transfer coefficient is commonly modeled by the dimensionless Nusselt number which expresses the ratio of total convective heat transfer to conductive heat transfer. The Nusselt number for a spherical particle is shown in Equation (3-40), where R_p is the particle's radius and κ_g is the thermal conductivity of the gas phase. Note that the Nusselt number's definition is similar that of the Biot number presented in Equation (3-4). However, the Nusselt number's definition uses the thermal conductivity of the fluid as opposed to the solid.

$$\text{Nu}_p = \frac{\gamma_{cp}}{\kappa_g/2R_p} \quad (3-40)$$

A large number of experimental correlations for the Nusselt number are available in the literature [69,70,71,72,73]. Typically, correlations are reported in a format similar to that presented in Equation (3-41) where a , b , c , and d are fitted empirical constants, and Re and Pr are the dimensionless Reynolds and Prandtl numbers, respectively. The Reynolds number, defined in Equation (3-42), is the ratio of inertial forces and viscous forces in the fluid. The Prandtl number, given by Equation (3-43), is the ratio of momentum and thermal diffusivity in the fluid. In these equations, ρ_g , ε_g , κ_g , C_{pg} , μ_g , and $\mathbf{v}_g$ are the density, void fraction, thermal conductivity, specific heat, viscosity, and velocity of the gas, respectively. R_p and $\mathbf{V}_p$ are the radius and velocity of the particle.

$$\text{Nu}_p = a + b\text{Re}^c\text{Pr}^d \quad (3-41)$$

$$\text{Re} = \frac{\rho_g \varepsilon_g \|\mathbf{v}_g - \mathbf{V}_p\|_2 2R_p}{\mu_g} \quad (3-42)$$

$$\text{Pr} = \frac{C_{pg}\mu_g}{\kappa_g} \quad (3-43)$$

Nusselt number correlations of the form shown in Equation (3-41) are assumed to include both *natural* and *forced convection*. Typically, natural convection (also referred to as *free convection*) is associated with a change in density of the fluid. For example, consider a hot object surrounded by a cooler fluid. The density of the fluid at near the object's surface decreases as heat is transferred to it from the object. The warmer, less dense fluid then rises, allowing cooler fluid to take its place at the objects surface. In contrast, forced convection occurs when fluid is moved past an object due to some external force (e.g., a free-falling particle, fan, pump, etc.). Thus, the constant a in Equation (3-41) captures the effects of natural convection as $Re \rightarrow 0$, while the second term in Equation (3-41) ($bRe^c Pr^d$) incorporates the contribution to heat transfer from forced convection as the Reynolds number increases.

Although numerous experimental correlations for the Nusselt number exist, this work employs the correlation of Ranz and Marshall [69], defined in the following section. The inclusion of additional correlations is addressed in Section 3.6.2.

3.4.2 Ranz and Marshall [69] (1952)

Ranz and Marshall's [69] correlation is given in Equation (3-44). This expression was developed by analyzing heat transfer data from evaporating water droplets, suspended in an upward-flowing gas. Recall that Re and Pr are the dimensionless Reynolds and Prandtl numbers defined in Equations (3-42) and (3-43), respectively.

$$Nu_p = 2.0 + 0.6Re^{1/2}Pr^{1/3} \quad (3-44)$$

Since Ranz and Marshall's [69] investigation analyzed data from isolated particles (i.e., $\varepsilon_g \rightarrow 1$ in Equation (3-42)), additional considerations are needed as the solids volume fraction ($\varepsilon_s = 1 - \varepsilon_g$) increases. For $Re > 10^2$, experimentally obtained heat

transfer data from fluidized beds was shown to agree reasonably well with Equation (3-44). However, as the Reynolds number decreases ($Re < 10$), Equation (3-44) is shown to over predict the heat transfer coefficient for a bed of particles [74]. Specifically, as the Reynolds number decreases, observed values for the Nusselt number for the bed drop below two, the theoretical minimum given by Equation (3-44) as $Re \rightarrow 0$. It is hypothesized that this is a result of reduced particle-gas contact as particles in a bed move closer together [74]. No bounds on void fraction were found in the literature indicating an acceptable range in which this model is applicable. Additionally, no bounds for the Reynolds and Prandtl numbers were provided by Ranz and Marshall [69], but several recommendations are found in the literature. Fan and Zhu [29] suggest that Equation (3-44) is applicable for $Re < 10^4$ and $Pr \geq 0.7$ encompassing most gas-solids flows. Li and Mason [17] claim Equation (3-44) provides acceptable results for $Re < 200$, while Mankad, Nixon, and Fryer [75] suggest it only applicable for $Re < 100$.

Ranz and Marshall's [69] correlation is employed in numerous CFD-DEM models [2,16,17,21,76] as well as a variation found in [18] (i.e., $Nu = 2\varepsilon_g + 0.69Re^{1/2}Pr^{1/3}$). Likewise, Equation (3-44) was selected as the *default* correlation for this work. The consideration to include additional correlations in the future is addressed in Section 3.6.2. This completes the discussion on particle-gas convective heat transfer. Here, Equation (3-39) is established as the convective heat transfer model ($\dot{Q}_{pg}$) for the particle internal energy equation (Equation (3-6)). Ranz and Marshall's [69] Nusselt number correlation (Equation (3-44)) was selected as the default closure model for the heat transfer coefficient (γ_{cp}) in Equation (3-39). The following section introduces particle-environment radiative heat transfer ($\dot{Q}_{rad}$) in gas-solids systems.

3.5 Particle-particle radiation

Radiative heat transfer occurs between the surfaces of solids [77] as well as an object's surface and the fluid surrounding it. Specifically, radiative heat transfer in gas-solids systems may occur between the particles and walls, individual/groups of particles, and the particles and gas. Presently, MFIX-DEM operates with the assumption that system walls are adiabatic (i.e., perfectly insulated so that no thermal energy enters or leaves the system through the walls). As a result, radiative heat transfer between particles and walls is not considered. Information concerning particle-wall heat transfer is found in references [29,78,79]. Additionally, this work assumes that the gas phase is *perfectly transparent* (i.e., the gas offers no resistance or contribution to radiative heat transfer). Therefore, particle-gas radiative heat transfer is also not considered. Information concerning particle-gas radiative heat transfer is provided in references [47,80]. Finally, particle-particle radiative heat transfer is commonly omitted from CFD-DEM heat transfer models [17,21,51,59,60,61,63,67,76,81] due to its negligible contribution to overall heat transfer at temperatures below 600°C [63]. However, as temperatures increase, the importance of particle-environment radiation also increases [19,78]. Since a goal of this work is to construct a comprehensive heat transfer model for the CFD-DEM, particle-particle radiative heat transfer is included for completeness. The negligible effect of radiative heat transfer at moderate temperatures is addressed in the implementation discussion.

This section continues by briefly describing radiative heat transfer, whereas the interested reader is directed to references [47,82] for a thorough review of the topic. The radiative heat transfer model employed in various CFD-DEM models is presented.

Finally, the distinguishing closer term separating these models , T_{env} (i.e., *environment temperature*), is discussed as well as the new definition developed for this work.

3.5.1 Background of particle-particle radiation

Radiative heat transfer is the result of reflecting, absorbing, and emitting of thermal radiation [47]. An object that absorbs all incident radiation (i.e., no radiation is reflected) is termed a *blackbody* or is said to have a *black surface*. The rate at which radiation is emitted from a blackbody per unit surface area (E_b) is called the blackbody emissive power and is given by the Stefan-Boltzmann law, shown as Equation (3-45). Here, σ is the Stefan-Boltzmann constant, and T is the temperature of the blackbody.

$$E_b = \sigma T^4 \quad (3-45)$$

Real surfaces absorb and emit less radiation than black surfaces. The *absorptance* (ς) is the fraction of incident radiation absorbed by a surface. Conversely, *reflectance* (ρ) is the fraction of incident radiation reflected by a surface. For surfaces that are not transparent, $\rho = 1 - \varsigma$. The *emittance* (ϵ) is the fraction of blackbody emissive power a surface possess (i.e., the ratio of actual to ideal emissive power). Typically, real surfaces are treated as *gray surfaces*, wherein the absorptance and emittance are equal ($\epsilon = \varsigma$ and $\epsilon = 1 - \rho$).

An energy balance between two diffuse, gray surfaces leads to Equation (3-46) (see reference [47] for details). Here, T , A_s , and ϵ are the temperatures, surface areas, and emittances of surfaces i and j , respectively. F_{ij} is the shape factor (also referred to as a *view factor*), which indicates the fraction of radiation emitted by surface i that is absorbed by surface j . Various configurations for surface factors are tabulated and available in an assortment of tables and graphs [47,83].

$$\dot{Q}_{rad}^{(i,j)} = \frac{\sigma T_j^4 - \sigma T_i^4}{\frac{1 - \epsilon_i}{\epsilon_i A_{si}} + \frac{1}{A_{si} F_{ij}} + \frac{1 - \epsilon_j}{\epsilon_j A_{sj}}} \quad (3-46)$$

The complexity of Equation (3-46) is reduced by considering the particles surrounding a particle of interest as a complete surface. Specifically, the neighboring particles are assumed to form a spherical environment surrounding the particle, as illustrated Figure 3-18. This reduces the multiple particle radiative heat transfer problem to one of concentric spheres ($F_{ij} = 1$ [47]). Furthermore, by assuming that the environment has a nearly black surface ($\epsilon_j \approx 1$), Equation (3-46) reduces to Equation (3-47). Observe that this simplification also arises by assuming that the surface area of the environment is sufficiently large (i.e., $A_{sj} \gg 1$).

Figure 3-18: A multi-particle radiation problem is reduced by assuming that the particles predominantly exposed to radiation form a spherical environment surrounding the particle of interest.

$$\dot{Q}_{rad}^{(i)} = \epsilon_i A_{si} \sigma (T_{env}^4 - T_i^4) \quad (3-47)$$

Various CFD-DEM codes use Equation (3-47) for modeling particle-particle radiative heat transfer [16,18,19,20]. The main distinction separating these models is their definitions for the environment temperature, T_{env} . Two definitions found in the literature

are discussed in the following section. Finally, a new definition for the environment temperature developed for this effort is presented.

3.5.2 Environment temperature definition

One definition for the environment temperature found in the literatures is obtained by averaging the temperature of *all particles* in a system [16,18,20], as shown in Equation (3-48). Here, N_p is the total number of particles in a simulation, and T_p is the temperature of the indexed particle. This definition invokes the assumption that every particle is exposed to the same radiative heat flux. For example, an isolated particle will experience the same radiative heat flux as a particle, at the same temperature, surrounded by several particles whose temperatures differ greatly from the average solids temperature. As a result, this definition is not employed in this work, in favor of one that computes T_{env} based upon the local conditions of a particle.

$$T_{env} = \frac{1}{N_p} \sum_{j=1}^{N_p} T_p^{(j)} \quad (3-48)$$

Zhou, Yu, and Zulli [19] calculate the environment temperature based on the contents of a sub-domain surrounding a particle. This is shown in Equation (3-49) and illustrated in Figure 3-19. In this equation, Ω defines the sub-domain around the i^{th} particle, $N_{p,\Omega}$ is the number of particles in the sub-domain, and ε_g and T_g are the void fraction and temperature of the gas, respectively. The authors define the radius of the sub-domain as 1.5 times the diameter of the particle. This definition addresses the limitation observed in Equation (3-48), however, by including the temperature of the gas, Equation (3-49) suggests some consideration to particle-gas radiative heat transfer is needed. Since

particle-gas radiative heat transfer is not considered in this work (see Section 3.5), this definition for the environment temperature was not selected.

$$T_{env}^{(i)} = \varepsilon_g T_{g,\Omega} + (1 - \varepsilon_g) \frac{1}{N_{p,\Omega}} \sum_{\substack{j=1 \\ j \neq i}}^{N_{p,\Omega}} T_p^{(j)} \quad (3-49)$$

Figure 3-19: Illustration of the sub-domain model proposed by Zhou, Yu, and Zulli [19] for determining the environment temperature used to calculate the rate of radiative heat transfer with particle i . In this example, three particles are in the sub-domain (i.e., $N_{p,\Omega} = 3$) of particle i .

In this effort, the environment temperature is defined as Equation (3-50). This definition considers the temperature of the surrounding particles and assumes negligible radiative heat transfer between the gas and particle. Note that Equation (3-50) is very similar to each of the above for environment temperature. That is, equating $N_{p,\Omega}$ to N_p in Equation (3-50) produces Equation (3-48), while setting $\varepsilon_g = 0$ in Equation (3-49) results in Equation (3-50).

$$T_{env}^{(i)} = \frac{1}{N_{p,\Omega}} \sum_{\substack{j=1 \\ j \neq i}}^{N_{p,\Omega}} T_p^{(j)} \quad (3-50)$$

This completes the discussion of particle-particle radiation ($\dot{Q}_{rad}$). Here, Equation (3-47) is established as the radiation heat transfer model ($\dot{Q}_{rad}$) for the particle internal

energy equation (Equation (3-6)). The environment temperature (T_{env}) needed for closer of Equation (3-47) is defined by Equation (3-50).

This section concludes the survey on the individual mechanisms of heat transfer considered in this work and the selection of a heat transfer model for each mechanism. The following section outlines the implementation of these models into MFIX-DEM.

3.6 Implementation of models

The mathematical models selected to describe the four forms of particle heat transfer considered in this effort and discussed in the preceding sections, are summarized in Table 3-1. These models were implemented into MFIX-DEM, an existing CFD-DEM code.

Table 3-1: Summary of the particle internal energy equation and four forms of particle heat transfer considered in this work.

particle internal energy equation (Section 3.1.3)	$m^{(i)} C_{pp}^{(i)} \frac{dT_p^{(i)}}{dt} = \dot{Q}_{pp}^{(i)} + \dot{Q}_{pfp}^{(i)} + \dot{Q}_{pg}^{(i)} + \dot{Q}_{rad}^{(i)}$
particle-particle contact conduction (Section 3.2.2)	$\dot{Q}_{pp}^{(i,j)} = \frac{4\kappa_p^{(i)}\kappa_p^{(j)}}{\kappa_p^{(i)} + \kappa_p^{(j)}} \sqrt{R_p^{(k)2} - \left(\frac{R_p^{(k)2} - R_p^{(l)2} + \ell^{(i,j)2}}{2\ell^{(i,j)}} \right)^2} (T_p^{(j)} - T_p^{(i)})$
particle-fluid-particle conduction (Section 3.3.2)	$\dot{Q}_{pfp}^{(i,j)} = \kappa_g (T_p^{(j)} - T_p^{(i)}) \int_{R_c}^{R_f^{(i,j)}} \frac{2\pi r}{\ell^{(i,j)} - \left((R_p^{(i)2} - r^2)^{1/2} + (R_p^{(j)2} - r^2)^{1/2} \right)} dr$ <p>where</p> $R_c = \begin{cases} 0 & \text{for } \ell^{(i,j)} > 2R_p \\ \sqrt{R_p^{(k)2} - \left(\frac{R_p^{(k)2} - R_p^{(l)2} + \ell^{(i,j)2}}{2\ell^{(i,j)}} \right)^2} & \text{for } \ell^{(i,j)} \leq 2R_p \end{cases}$ <p>and</p> $R_p^{(k)} = \max\{R_p^{(i)}, R_p^{(j)}\} \quad \text{and} \quad R_p^{(l)} = \min\{R_p^{(i)}, R_p^{(j)}\}$
particle-gas convection (Sections 3.4.1 and 3.4.2)	$\dot{Q}_{pg} = \gamma_{cp} A_s (T_g - T_p) \quad \text{where} \quad \text{Nu}_p = \frac{\gamma_{cp}}{\kappa_g/2R_p} = 2.0 + 0.6\text{Re}^{1/2}\text{Pr}^{1/3}$
particle-particle radiation (Sections 3.5.1 and 3.5.2)	$\dot{Q}_{rad}^{(i)} = \epsilon_i A_{si} \sigma (T_{env}^4 - T_i^4) \quad \text{where} \quad T_{env}^{(i)} = \frac{1}{N_{p,\Omega}} \sum_{\substack{j=1 \\ j \neq i}}^{N_{p,\Omega}} T_p^{(j)}$

This required the modification and creation of several subroutines. Descriptions of new subroutines are outlined in Table 3-2, while the source code is reserved for Appendix D. Modifications to existing routines mainly consist of logical checks associated with call statements to the new routines. A call-tree showing the invocation of the heat transfer model initialization routines is shown in Figure 3-20, and the invocation of the heat transfer model operational routines is shown by the call-tree in Figure 3-21.

Table 3-2: A list of subroutines developed to set initial conditions of particles and manage the heat transfer models implemented into MFIX.

Subroutine <i>file name</i>	Description
DES_IC <i>des_ic_mod.f</i>	Global data storage for common initial condition data.
CHECK_DES_IC <i>check_des_ic.f</i>	Checks the data provided for the DES initial conditions and flag errors if data is improper.
DES_SET_IC <i>des_set_ic.f</i>	Assigns the necessary data (e.g., temperature) to each particle at the start of a simulation.
DES_THERMO <i>des_thermo_mod.f</i>	Global data storage for the heat transfer model.
CHECK_DES_THERMO <i>check_des_thermo.f</i>	Checks the data provided for the heat transfer model, and sets various flags used by the heat transfer implementation.
CALC_THERMO_DES <i>calc_thermo_des.f</i>	Calls the routines that calculate the various heat transfer models.
DES_CONDUCTION <i>des_thermo_cond.f</i>	Calculates the rate of heat transfer resulting from contact conduction and particle-fluid-particle heat transfer.
DES_CONVECTION <i>des_thermo_conv.f</i>	Calculates the rate of heat transfer between the particle and the gas acting on the particle.
DES_Hgm <i>des_thermo_conv.f</i>	Calculates the rate of heat transfer between particles and the gas acting on the gas.
DES_CALC_GAMMA <i>des_thermo_conv.f</i>	Calculates the heat transfer coefficient based on the specified Nusselt number model.
DES_RADIATION <i>des_thermo_rad.f</i>	Calculates the rate of particle-environment radiative heat transfer.
DES_THERMO_NEWVALUES <i>des_thermo_newvalues.f</i>	Advances the solution of the internal energy equation for a particle through numerical integration.

THERMO_NBR <i>thermo_nbr.f</i>	Determines if a particle belongs in the thermodynamic neighborhood of another particle. This subset of particles is used to assess which particles are undergoing contact conduction and radiative heat transfer.
INTERPOLATE_CC <i>interpolation_mod.f</i>	Populates the variables needed for interpolating data from the Eulerian grid to a particle's position.
SET_INTERPOLATION_STENCIL_CC <i>interpolation_mod.f</i>	Calculates the indices needed to access the Eulerian grid cells for interpolation.

Figure 3-20: Call graph of main MFIX-DEM source code for initialization routines. Dashed lines indicate new calls and subroutines implemented for the heat transfer model.

Figure 3-21: Call graph of MFX discrete particle model routines. Dashed lines indicate new calls and subroutines implemented for the heat transfer model.

A flow chart depicting the heat transfer algorithm implemented in MFX-DEM is presented in Figure 3-22. Processes added to the original DEM algorithm are indicated by dashed lines. The implementation is generalized by allowing a *user* to omit any mode of heat transfer he/she deems negligible by setting specific flags in the setup file (i.e., mfix.dat [84]). For example, a user may turn off radiative heat transfer in a simulation operating below 600°C to reduce computational expense. A flowchart detailing the processes for calculating the particle heat fluxes is illustrated in Figure 3-23. Discussions

addressing interpolation and updating a particle's temperature are reserved for Sections 3.6.1 and 3.6.3, respectively.

Figure 3-22: Flow chart illustrating the locations within MFIx-DEM where modifications have been made to include particle heat transfer.

Figure 3-23: Flow chart illustrating customizability of the implementation by allowing a user to select which modes of heat transfer to compute during a simulation.

3.6.1 Gas-solids thermal energy transfer

Particle-gas convection, $\dot{Q}_{pg}$, introduced in Section 3.4, is an interphase heat transfer term that couples the gas and particle energy balance equations. Specifically, particle-gas convection is a source term in the internal energy equations for the gas (q_{gs} in Equation (1-6)) and particle ($\dot{Q}_{pg}$ in Equation (3-6)). In MFIX the numerical solution of the gas phase energy equation separates $\dot{Q}_{pg}$ into the coefficient for the *unknown* gas

phase temperature ($-\gamma_{cp}A_s$) and a *known* source term ($\gamma_{cp}A_sT_p$). (See references [85,86] for detailed solution methodology used in MFIX for continuum phases).

A consistent approach is needed to manage thermal energy transfer between the particles and gas (i.e., how information is transferred between the Eulerian grid and discrete particles). For example, gas phase temperature is a scalar variable associated with the Eulerian grid cell centers. However, particles can exist in any region of the domain defined by the Eulerian grid, as illustrated in Figure 3-24. Therefore, passing energy (information) between the Eulerian grid and particles can occur through either a direct exchange between a particle and the Eulerian cell that contains its center, or through interpolating the information to the nearest Eulerian cells surrounding the particle.

Figure 3-24: Example illustrating the Eulerian grid which stores scalar field variables, like temperature, at the cell-center. Particles are permitted to exist at any location within the domain defined by the Eulerian grid.

Equation (3-51) defines the particle-gas convective heat transfer acting on the gas phase, q_{gs} . Here, $\mathcal{V}_{CV}$ is the volume of the control volume (CV), N_{CV} is the number of particles contained in the CV, and $\dot{Q}_{pg}$ is the rate of particle-gas convective heat transfer given by Equation (3-39) and relations (3-40) and (3-44). $K_{CV}^{(k)}$ is a function used to map the energy flux from a particle's position to the computational nodes of the gas phase Eulerian grid.

$$q_{gs} = -\frac{1}{V_{CV}} \sum_{k=1}^{N_{CV}} \dot{Q}_{pg}^{(k)} K_{CV}^{(k)} \quad (3-51)$$

Presently, there are two definitions for the mapping function, $K_{CV}^{(k)}$. By default, thermal energy transfer between the fluid and a particle is associated with the CV containing the particle's center, as illustrated in Figure 3-25-(a). Therefore, calculations that require the temperature of the gas phase (i.e., Equation (3-39)) use the temperature associated with the CV (fluid cell) containing the particle's center. Also, thermal energy taken from, or given to the fluid as the result of particle-gas convective heat transfer is done so with the fluid cell containing the particle's center. A second option distributes thermal energy flux among the control volumes surrounding the particle via linear interpolation. This technique is depicted in Figure 3-25-(b). If the interpolation method is employed, the gas phase temperature used in Equation (3-39) is interpolated to a particle's position from the surrounding control volumes for consistency. Likewise, thermal energy transfer resulting from particle-gas convective heat transfer is distributed among the control volumes surrounding the particle.

Figure 3-25: Example illustrating the two methods available to transmitting thermal energy between the Eulerian grid and the particles. (a) Energy is passed between a particle and the grid cell containing its center; (b) energy is distributed from a particle's position to the nearest grid cells.

Finally, one must consider when information is exchanged between the gas and particles. This is a result of the solution technique used to computationally join the gas and discrete solids phases. Presently in MFIX-DEM [85], the gas phase takes a step forward in time using an extended version of the SIMPLE algorithm [86] (not presented). Once the fluid variables converge, several smaller time steps are taken within the DEM to allow the particles to catch-up to the gas phase [35]. This *fluid step forward-particle catch-up* process is illustrated in Figure 3-26.

Figure 3-26: Illustration of the fluid step forward-particle catch-up process that occurs during MFIX-DEM. First the solution to the fluid phase is obtained at time t , then multiple, smaller time steps are taken within the DEM to allow the particles to catch-up to the fluid phase. Here, t is the time of the fluid's most recent solution, and t_s is the time of the discrete solids most recent solution.

The source terms for the internal energy equations for the particles and gas are managed differently to account for the disjoint updating procedure. When the gas phase equations are solved, *all* of the physical properties of the particles are constant. This is a direct result of their solutions lagging behind the solution of the gas phase. Furthermore, only the coefficient for the *unknown* gas phase temperature $\left(\frac{-1}{V_{CV}} \sum_{k=1}^{N_{CV}} \gamma_{cp} A_s^{(k)} K_{CV}^{(k)}\right)$ and the *known* source term $\left(\frac{-1}{V_{CV}} \sum_{k=1}^{N_{CV}} \gamma_{cp} A_s^{(k)} T_p^{(k)} K_{CV}^{(k)}\right)$ are computed for each fluid cell (see Equations (3-39) and (3-51), subroutine DES_Hgm in Appendix 0, and references [85,86]). Similarly, when the particle phase equations are solved, *all* of the physical properties of the gas phase are constant, and only the contributions to the particle internal energy equation are calculated ($\dot{Q}_{pg}$ in Equation (3-6)).

3.6.2 Nusselt number correlations

The model for particle-gas convection, introduced in Section 3.4, requires a closure model for the heat transfer coefficient, γ_{cp} . Ranz and Marshall's [69] correlation, discussed in Section 3.4.2, was selected as the *default* Nusselt number correlation for this work, however, numerous correlations are available in the literature [69,70,71,72,73]. To provide greater customizability of the convective heat transfer model, a general framework was created to facilitate implementation of additional correlations by users. This was achieved by providing a set location within the code (see subroutine DES_CALC_GAMMA in Appendix 0) for the user to implement their correlation. By creating a flag in the setup file (i.e., mfix.dat [84]) a user may indicate which correlation to use during a simulation. This approach allows for multiple correlations to exist within the code simultaneously, while only evaluating the desired correlation during execution.

3.6.3 Temperature updating procedures

There are various methodologies available for solving differential equations numerically[87,88,89]. However, the time integration methods for the discrete solids phase momentum equation implemented in MFIX-DEM are limited to Euler's and Adams-Bashforth methods [35]. Therefore, the same methods were used to advance the solution of the particle internal energy equation. Euler's method, shown as Equation (3-52), is the default approach selected by this work. However, the Adams-Bashforth method (not shown) is available for higher accuracy. Details concerning these methods are provided in references [88,89].

$$T_p^{(i)}(t + \Delta t_s) = T_p^{(i)}(t) + \frac{\Delta t_s}{m^{(i)}(t)c_{pp}^{(i)}(t)} \left(\dot{Q}_{pp}^{(i)}(t) + \dot{Q}_{pfp}^{(i)}(t) + \dot{Q}_{pg}^{(i)}(t) + \dot{Q}_{rad}^{(i)}(t) \right) \quad (3-52)$$

The step size for the numerical integration of the particle internal energy equation, Δt_s , is the same used for the numerical integration of the particle momentum equation. Although the solids time step for numerical stability of the collision model is orders of magnitude more smaller than that needed for stability of the particle internal energy (see Section 3.2.3), the same solids time step is used.

3.6.4 Integral management in particle-fluid-particle conduction model

The particle-fluid-particle conduction model, discussed in Section 3.3.2, contains an integral which represents the heat transfer paths joining the surfaces of the particles. A numerical approach is needed to solve the integral, shown in Equation, as no analytical solution is obvious.

$$\int_{R_c}^{R_f^{(i,j)}} f(r) dr \quad \text{where} \quad f(r) = \frac{2\pi r}{\ell^{(i,j)} - \left(\left(R_p^{(i)^2} - r^2 \right)^{1/2} + \left(R_p^{(j)^2} - r^2 \right)^{1/2} \right)} \quad (3-53)$$

As noted in the discussion in Section 3.3.2, a singularity in Equation (3-53) occurs as $\ell^{(i,j)}$ approaches zero. The singularity is avoid in this effort by requiring a minimum separation distance between particles' surfaces of 4×10^{-10} m. However, the slope of $f(r)$ varies sharply across integral bounds, resulting in additional difficulty. Adaptive Simpson's method [88] (see subroutine DES_CONDUCTION in Appendix 0) was selected to numerically integrate this term due to its ability to compute the value quickly while maintaining a known bound on the amount of error generated.

3.7 Verification of implementation

In this section, implementation of the contact conduction, particle-fluid-particle conduction, and particle-gas convection models in MFIX-DEM are verified by comparing the numerical results to analytic solutions. Simple test cases were developed

to isolate the heat transfer mechanisms of interest. Recall from Section 3.6, a simulation may selectively omit individual mechanisms of heat transfer. Implementation of the particle-particle radiation model is verified by comparing the results of MFIX-DEM with those of a fourth order Runge-Kutta (RK4) solution. An analytic solution for particle-particle radiation was not sought due to a nonlinear dependence on particle temperatures (see Equation set (3-61)).

3.7.1 Contact conduction

Implementation of the contact conduction model (see Section 3.2.2) was verified using the case of two touching particles. The particles' positions are assumed fixed in time and heat transfer is assumed to occur only via particle-particle conduction. In this case the internal energy equation for each particle (see Equation (3-6)) reduces to the expressions shown in Equation set (3-54) describing the temperatures of particles indexed by the numbers 1 and 2. Here, m , C_{pp} , κ_p , R_p , and T_p are the mass, specific heat, thermal conductivity, radius, and temperatures of the indexed particles, respectively.

$$\begin{aligned}\frac{dT_p^{(1)}}{dt} &= \frac{4\kappa_p^{(1)}\kappa_p^{(2)}(T_p^{(2)} - T_p^{(1)})}{m^{(1)}C_{pp}^{(1)}(\kappa_p^{(1)} + \kappa_p^{(2)})} \sqrt{R_p^{(2)2} - \left(\frac{R_p^{(2)2} - R_p^{(1)2} + \ell^{(2,1)2}}{2\ell^{(1,2)}}\right)^2} \\ \frac{dT_p^{(2)}}{dt} &= \frac{4\kappa_p^{(2)}\kappa_p^{(1)}(T_p^{(1)} - T_p^{(2)})}{m^{(2)}C_{pp}^{(2)}(\kappa_p^{(2)} + \kappa_p^{(1)})} \sqrt{R_p^{(2)2} - \left(\frac{R_p^{(2)2} - R_p^{(1)2} + \ell^{(2,1)2}}{2\ell^{(2,1)}}\right)^2}\end{aligned}\tag{3-54}$$

An analytic solution for the particles' temperature is obtained for particles with constant (but not necessarily equal) thermal and physical properties (m , C_{pp} , κ_p , and R_p). The resulting system of ordinary differential equations is solved by diagonalization. The

solutions for the particles' temperatures as a function of time are shown as Equation set (3-55). Here, $T_{p,0}$ is the initial temperature of the indexed particles, respectively.

$$\begin{aligned}
T_p^{(1)}(t) &= \frac{1}{a+b} \left[bT_{p,0}^{(1)} + aT_{p,0}^{(2)} + a \left(T_{p,0}^{(1)} - T_{p,0}^{(2)} \right) e^{-(a+b)t} \right], \\
T_p^{(2)}(t) &= \frac{1}{a+b} \left[bT_{p,0}^{(1)} + aT_{p,0}^{(2)} - b \left(T_{p,0}^{(1)} - T_{p,0}^{(2)} \right) e^{-(a+b)t} \right], \\
\text{where } a &= \frac{2}{m^{(1)}C_{pp}^{(1)}} \left(\frac{\kappa_p^{(1)}\kappa_p^{(2)}}{\kappa_p^{(1)} + \kappa_p^{(2)}} \right) \sqrt{R_p^{(2)2} - \left(\frac{R_p^{(2)2} - R_p^{(1)2} + \ell^{(2,1)2}}{2\ell^{(1,2)}} \right)^2}, \\
\text{and } b &= \frac{2}{m^{(2)}C_{pp}^{(2)}} \left(\frac{\kappa_p^{(1)}\kappa_p^{(2)}}{\kappa_p^{(1)} + \kappa_p^{(2)}} \right) \sqrt{R_p^{(2)2} - \left(\frac{R_p^{(2)2} - R_p^{(1)2} + \ell^{(2,1)2}}{2\ell^{(2,1)}} \right)^2}.
\end{aligned} \tag{3-55}$$

A simulation employing the same assumptions defined above was conducted with MFIX-DEM where only particle-particle conduction was solved. The physical and thermodynamic properties of the particles are outlined in Table 3-3, and illustrated in Figure 3-27. The values are based on those used in reference [19] who studied heat transfer in packed and bubbling beds using CFD-DEM. In this simulation, 1000 seconds of physical time was modeled to allow the particles to achieve an equilibrium temperature ($|\Delta T_p| \leq 10^{-4}$). The solids time step was kept constant at $\Delta t_s = 0.856357 \times 10^{-6}$. A single AMD Opteron 265, 1.8GHz processor was used.

Table 3-3: Physical and thermodynamic properties of the particles used to verify the contact conduction model implemented into MFIX-DEM. The geometric configuration is illustrated in Figure 3-27.

properties	particle 1	particle 2
diameter (cm)	0.30	0.36
density (g/cm ³)	0.42	8.85
thermal conductivity (cal/sec·cm·K)	0.131453	0.002008

specific heat (cal/g·K)	0.191204	0.013145
initial temperature (K)	298.15	453.15
x-position (cm)	2.5	2.5
y-position (cm)	0.1499864	0.4799731
z-position (cm)	0.18	0.18

Figure 3-27: The geometric configuration of the particles used to verify the implementation of the contact conduction model implemented into MFIX-DEM. All measurements are in centimeters.

The numerical and analytical solutions for the particles' temperatures are shown in Figure 3-28. T_{p1} and T_{p2} indicate the temperatures of particle 1 particle 2, respectively. Solid symbols denote the particle temperatures calculated by MFIX-DEM, continuous lines represent the analytic solutions, and open symbols indicate the percent relative error between the numerical and analytical solutions as defined in Equation (3-56). Note the strong agreement between the analytic and numerical solutions. Percent relative error is bounded above by 10^{-5} , indicating the numerical solution deviates less than $\pm 10^{-5}$ percent from the analytic solution over the entire simulation. Therefore, the implementation of the contact conduction model into the MFIX-DEM code is considered successful.

Figure 3-28: MFIX-DEM and analytic solutions to the internal energy equation for two particles engaged in contact conduction. Tp1 and Tp2 are the temperatures of the cold and hot particles, respectively. Relative error between the analytic and numerical solutions is indicated by open symbols and is associated with the right vertical axis.

$$\text{Percent Relative Error} = \frac{|T_{pk}^{\text{analytic}} - T_{pk}^{\text{MFIX-DEM}}|}{|T_{pk}^{\text{analytic}}|} \times 100\% \quad (3-56)$$

3.7.2 Particle-fluid-particle conduction

Implementation of the particle-fluid-particle conduction model (see Section 3.3.2) was verified using the same test case as in the particle-particle conduction verification study but with an additional variation. Specifically, two test cases were constructed. In the first test case, the two particles are close but not in contact, while in the second test, the particles are touching. The particles' positions are assumed fixed in time and heat transfer is assumed to occur only via particle-fluid-particle conduction. In this case the internal energy equation for each particle (see Equation (3-6)) reduces to the expressions shown in Equation set (3-57) describing the temperatures of particles indexed by the numbers 1 and 2. Here, κ_g is the thermal conductivity of the gas, and m , C_{pp} , R_p , and T_p

are the mass, specific heat, radius, and temperatures of the indexed particles, respectively.

R_f and R_c delineate the region of particle-fluid-particle conduction, and are defined in Equations (3-25), (3-36), and (3-37), respectively.

$$\begin{aligned}\frac{dT_p^{(1)}}{dt} &= \frac{\kappa_g (T_p^{(2)} - T_p^{(1)})}{m^{(1)} C_{pp}^{(1)}} \int_{R_c}^{R_f^{(1,2)}} \frac{2\pi r}{\ell^{(1,2)} - \left((R_p^{(1)})^2 - r^2 \right)^{1/2} + \left((R_p^{(2)})^2 - r^2 \right)^{1/2}} dr \\ \frac{dT_p^{(2)}}{dt} &= \frac{\kappa_g (T_p^{(1)} - T_p^{(2)})}{m^{(2)} C_{pp}^{(2)}} \int_{R_c}^{R_f^{(1,2)}} \frac{2\pi r}{\ell^{(1,2)} - \left((R_p^{(2)})^2 - r^2 \right)^{1/2} + \left((R_p^{(1)})^2 - r^2 \right)^{1/2}} dr\end{aligned}\quad (3-57)$$

As before, analytic solutions for the particles' temperature are obtained for particles and gas with constant thermal and physical properties (m , C_{pp} , κ_p , R_p , and κ_g). These assumptions result in a system of ordinary differential equations solved by diagonalization. The resulting solutions for the particles' temperatures are shown in Equation set (3-58). Here, $T_{p,0}$ is the initial temperature of the indexed particles.

$$\begin{aligned}T_p^{(1)}(t) &= \frac{1}{a+b} \left[bT_{p,0}^{(1)} + aT_{p,0}^{(2)} + a(T_{p,0}^{(1)} - T_{p,0}^{(2)}) e^{-(a+b)t} \right], \\ T_p^{(2)}(t) &= \frac{1}{a+b} \left[bT_{p,0}^{(1)} + aT_{p,0}^{(2)} - b(T_{p,0}^{(1)} - T_{p,0}^{(2)}) e^{-(a+b)t} \right],\end{aligned}$$

where
$$a = \frac{\kappa_g}{m^{(1)} C_{pp}^{(1)}} \int_{R_c}^{R_f} \frac{2\pi r}{\ell^{(i,j)} - \left((R_p^{(1)})^2 - r^2 \right)^{1/2} + \left((R_p^{(2)})^2 - r^2 \right)^{1/2}} dr, \quad (3-58)$$

and
$$b = \frac{\kappa_g}{m^{(2)} C_{pp}^{(2)}} \int_{R_c}^{R_f} \frac{2\pi r}{\ell^{(i,j)} - \left((R_p^{(1)})^2 - r^2 \right)^{1/2} + \left((R_p^{(2)})^2 - r^2 \right)^{1/2}} dr.$$

Simulations with the same assumptions used to construct the analytic solutions were conducted with MFIX-DEM. Accordingly, only particle-fluid-particle convection was solved. The physical and thermodynamic properties of the particles are outlined in

Table 3-4, with the geometric configurations of the simulations illustrated in Figure 3-27 and Figure 3-25, respectively. The thermal conductivity of the gas was defined as 1.239×10^{-4} cal/sec·cm·K. As in the previous test case, all values follow from reference [19]. In the first simulation, 300 seconds of physical time was modeled to allow two non-touching particles to achieve an equilibrium temperature ($\Delta T_p \leq 10^{-4}$). Similarly, the second simulation, with touching particles, modeled 50 seconds of physical time to allow the particles to achieve an equilibrium temperature. The integral term in Equation (3-37) and Equation set (3-58) was evaluated using adaptive Simpsons quadrature [88]. The solids time step was kept constant $\Delta t_s = 0.856357 \times 10^{-6}$. Both simulations were carried out on a single AMD Opteron 265, 1.8GHz processor.

Table 3-4: Physical and thermodynamic properties of the particles used to verify the particle-fluid-particle conduction model implemented into MFI-X-DEM. The geometric configuration for the first simulation is illustrated in Figure 3-29 while the geometric configuration for the second simulation is illustrated in Figure 3-27. The gas phase thermal conductivity for both simulations was set as 1.239×10^{-4} cal/sec·cm·K.

properties	particle 1		particle 2	
diameter (cm)	0.30		0.36	
density (g/cm ³)	0.42		8.85	
thermal conductivity (cal/sec·cm·K)	0.131453		0.002008	
specific heat (cal/g·K)	0.191204		0.013145	
initial temperature (K)	298.15		453.15	
Simulation	1	2	1	2
x-position (cm)	2.5	2.5	2.5	2.5
y-position (cm)	1.15	1.1499864	1.498	0.4799731
z-position (cm)	0.18	0.18	0.18	0.18

Figure 3-29: The geometric configuration of the particles used in the first simulation to verify the implementation of the particle-fluid-particle conduction model implemented into MFIX-DEM. All measurements are in centimeters.

The numerical and analytical solutions for the particles' temperatures are shown in Figure 3-30 for the non-touching case and in Figure 3-31 for the touching case, respectively. T_{p1} and T_{p2} indicate the temperatures of particle 1 and particle 2, respectively. Solid symbols denote the particle temperatures calculated by MFIX-DEM, continuous lines represent the analytic solutions, and open symbols indicate the percent relative error between the numerical and analytical solutions (see Equation (3-56)). Note the strong agreement between the analytic and numerical solutions. For both test cases, percent relative error is bounded above by 10^{-5} , indicating the numerical solutions deviate less than $\pm 10^{-5}$ percent from the analytic solutions over the entire simulations. Therefore, the implementation of the particle-fluid-particle conduction model into the MFIX-DEM code is considered successful.

Figure 3-30: MFIX-DEM and analytic solutions to the internal energy equation for two particles not touching and engaged in particle-fluid-particle conduction. Tp1 and Tp2 are the temperatures of particle 1 and particle 2, respectively (c.f. Table 3-4). Relative error between the two solutions is indicated by open symbols and is associated with the right vertical axis.

Figure 3-31: MFIX-DEM and analytic solutions to the internal energy equation for two touching particles engaged in particle-fluid-particle conduction. Tp1 and Tp2 are the temperatures of particle 1 and particle 2, respectively (c.f. Table 3-4). Relative error between the two solutions is indicated by open symbols and is associated with the right vertical axis.

3.7.3 Particle-gas convection

Implementation of the particle-gas convection model (see Section 3.4) was verified using the case of a single particle fixed in a uniform gas flow. The particle's position is assumed fixed in time and heat transfer is assumed to occur only via particle-gas convection. In this case the internal energy equation for the particle (see Equation (3-6)) reduces to the expression shown in Equation (3-59) describing the temperature of particle. Here, κ_g , ρ_g , C_{pg} , μ_g , ε_g , T_g , and $\mathbf{v}_g$ are the thermal conductivity, density, specific heat, viscosity, void fraction, temperature, and velocity of the gas phase, and m , C_{pp} , R_p , A_s , T_p , and $\mathbf{V}_p$ are the mass, specific heat, radius, surface area, temperature, and velocity of the particle, respectively.

$$\frac{dT_p}{dt} = \frac{\gamma_{cp} A_s (T_g - T_p)}{m C_{pp}} \quad (3-59)$$

where $\gamma_{cp} = \frac{\kappa_g}{2R_p} \left(2.0 + 0.6 \left(\frac{\rho_g \varepsilon_g \|\mathbf{v}_g - \mathbf{V}_p\|_2 2R_p}{\mu_g} \right)^{1/2} \left(\frac{C_{pg} \mu_g}{\kappa_g} \right)^{1/3} \right)$

As before, an analytic solution for the particle's temperature is obtained for a particles and gas with constant thermal and physical properties (m , C_{pp} , R_p , A_s , $\mathbf{V}_p$, κ_g , ρ_g , C_{pg} , μ_g , ε_g , T_g , $\mathbf{v}_g$). These assumptions result in a ordinary differential solved by separation of variables. The resulting solution for the particle's temperature is shown in Equation (3-60), where $T_{p,0}$ is the particle's initial temperature.

$$T_p(t) = T_g - (T_g - T_{p,0}) e^{\frac{-\gamma_{cp} A_s}{m C_{pp}} t} \quad (3-60)$$

where $\gamma_{cp} = \frac{\kappa_g}{2R_p} \left(2.0 + 0.6 \left(\frac{\rho_g \varepsilon_g \|\mathbf{v}_g - \mathbf{V}_p\|_2 2R_p}{\mu_g} \right)^{1/2} \left(\frac{C_{pg} \mu_g}{\kappa_g} \right)^{1/3} \right)$

A simulation employing the same assumptions defined above was conducted with MFIX-DEM where only particle-gas convection was solved. The physical and thermodynamic properties of the particle and gas are outlined in Table 3-5, and illustrated in Figure 3-32. As in the previous test cases, all values follow from reference [19]. The simulation was run for 25 seconds of physical time to allow the particle's temperature to equilibrate with the gas temperature ($|T_p - T_g| \leq 10^{-4}$). The solids time step was kept constant $\Delta t_s = 0.856357 \times 10^{-6}$. The simulation was performed on a single AMD Opteron 265, 1.8GHz processor.

Table 3-5: Physical and thermodynamic properties of the gas and particle used to verify the convection model implemented into MFIX-DEM. The geometric configuration is illustrated in Figure 3-32.

properties	gas	particle
diameter (cm)	-	0.36
density (g/cm ³)	1.1854x10 ⁻³	8.85
thermal conductivity (cal/sec·cm·K)	1.2396x10 ⁻⁴	0.002008
specific heat (cal/g·K)	0.23878	0.013145
initial temperature (K)	298.15	453.15
velocity (cm/sec)	600	0

Figure 3-32: The geometric configuration of a particle used to verify the implementation of the particle-gas convection model implemented into MFIX-DEM. All measurements are in centimeters.

The numerical and analytical solutions for the particle's temperature is shown in Figure 3-33. T_p and T_g indicate the temperatures of the particle and gas, respectively. Solid symbols denote the particle's temperature calculated by MFIX-DEM, a continuous line represents the analytic solution for the particle's temperature, and open symbols indicate the percent relative error (see Equation (3-56)). The constant gas phase temperature is indicated with a dashed line. Note the strong agreement between the analytic and numerical solutions. Percent relative error is bounded above by 10^{-5} , indicating the numerical solution deviates less than $\pm 10^{-5}$ percent from the analytic solution over the entire simulation. Therefore, the implementation of the particle-gas convection model into the MFIX-DEM code is considered successful.

Figure 3-33: MFIX-DEM and analytic solutions to the internal energy equation for a single particle undergoing particle-gas convection with a constant fluid. T_p and T_g are the temperatures of particle and gas, respectively. Relative error between the numerical and analytic solutions is indicated by open symbols and is associated with the right vertical axis.

3.7.4 Particle-particle radiation

Implementation of the radiative heat transfer model (see Section 3.5) was verified using the case of two particles in close proximity to one another. The particles' positions are assumed fixed in time and heat transfer is assumed to occur only via particle-particle radiation. In this case the internal energy equation for each particle (see Equation (3-6)) reduces to the expressions shown in Equation set (3-61) describing the temperatures of particles indexed by the numbers 1 and 2. Here, σ is the Stefan-Boltzmann constant, and m , C_{pp} , ϵ , A_s , and T_p are the mass, specific heat, emissivity, surface area, and temperatures of the indexed particles, respectively.

$$\begin{aligned}\frac{dT_p^{(1)}}{dt} &= \sigma_{S-B} \frac{A_s^{(1)} \epsilon_p^{(1)}}{m^{(1)} C_{pp}^{(1)}} \left((T_p^{(2)})^4 - (T_p^{(1)})^4 \right) = f_1(t, T_p^{(1)}, T_p^{(2)}) \\ \frac{dT_p^{(2)}}{dt} &= \sigma_{S-B} \frac{A_s^{(2)} \epsilon_p^{(2)}}{m^{(2)} C_{pp}^{(2)}} \left((T_p^{(1)})^4 - (T_p^{(2)})^4 \right) = f_2(t, T_p^{(1)}, T_p^{(2)})\end{aligned}\tag{3-61}$$

Due to the nonlinear dependence on particle temperature, obtaining analytic solutions for the temperature of the particles is nontrivial. Therefore, a standard fourth-order Runge-Kutta (RK4) method, shown as Equation set (3-62) with time step $h = 10^{-3}$ and constant thermal and physical properties (m , C_{pp} , κ_p , and R_p), is used for comparison.

$$\begin{cases} T_p^{(1)}(t_{n+1}) = T_p^{(1)}(t_n) + \frac{1}{6}(k_1^{(1)} + 2k_2^{(1)} + 2k_3^{(1)} + k_4^{(1)}) & \text{where } T_p^{(1)}(t_0) = T_{p0}^{(1)} \\ T_p^{(2)}(t_{n+1}) = T_p^{(2)}(t_n) + \frac{1}{6}(k_1^{(2)} + 2k_2^{(2)} + 2k_3^{(2)} + k_4^{(2)}) & \text{where } T_p^{(2)}(t_0) = T_{p0}^{(2)} \end{cases}$$

where

$$\begin{cases} k_1^{(i)} = hf_i(t_n, T_p^{(1)}(t_n), T_p^{(2)}(t_n)) \\ k_2^{(i)} = hf_i\left(t_n + \frac{h}{2}, T_p^{(1)}(t_n) + \frac{k_1^{(1)}}{2}, T_p^{(2)}(t_n) + \frac{k_1^{(2)}}{2}\right) \\ k_3^{(i)} = hf_i\left(t_n + \frac{h}{2}, T_p^{(1)}(t_n) + \frac{k_2^{(1)}}{2}, T_p^{(2)}(t_n) + \frac{k_2^{(2)}}{2}\right) \\ k_4^{(i)} = hf_i\left(t_n + h, T_p^{(1)}(t_n) + k_3^{(1)}, T_p^{(2)}(t_n) + k_3^{(2)}\right) \end{cases} \quad \text{for } i \in \{1,2\} \quad (3-62)$$

A simulation employing the same assumptions defined above was conducted with MFIX-DEM where only particle-particle radiation was solved. The physical and thermodynamic properties of the particle and gas are outlined in Table 3-6, and illustrated in Figure 3-34. As in the previous test cases, all values follow from reference [19]. The simulation was run for 145 seconds of physical time to allow the particles to achieve an equilibrium temperature ($\Delta T_p \leq 10^{-4}$). The solids time step was kept constant $\Delta t_s = 0.856357 \times 10^{-6}$. The simulation was performed on a single AMD Opteron 265, 1.8GHz processor.

Table 3-6: Physical and thermodynamic properties of the particles used to verify the radiative heat transfer model implemented into MFIX-DEM. The geometric configuration is illustrated in Figure 3-34.

properties	particle 1	particle 2
diameter (cm)	0.30	0.36
density (g/cm ³)	0.42	8.85
thermal conductivity (cal/sec·cm·K)	0.131453	0.002008
specific heat (cal/g·K)	0.191204	0.013145
emissivity	0.8	0.8
initial temperature (K)	298.15	453.15
x-position (cm)	2.5	2.5

y-position (cm)	3.0	3.43
z-position (cm)	0.18	0.18

Figure 3-34: The geometric configuration of the particles used in the first simulation to verify the implementation of the particle-environment radiation model implemented into MFIX-DEM. All measurements are in centimeters.

The numerical and RK4 solutions for the particles' temperatures are shown in Figure 3-35.. Tp1 and Tp2 indicate the temperatures of particle 1 and particle 2, respectively. Solid symbols denote the particle temperatures calculated by MFIX-DEM, continuous lines represent the RK4 solutions, and open symbols indicate the percent relative error (see Equation (3-56)). Note the strong agreement between the RK4 and numerical solutions. The percent relative error is bounded above by 10^{-6} , indicating the numerical solutions deviate less than $\pm 10^{-5}$ percent from the RK4 solution over the entire simulation. Therefore, the implementation of the particle-particle radiation model into the MFIX-DEM code is considered successful.

Figure 3-35: MFIX-DEM and fourth order Runge-Kutta (RK4) solutions to the internal energy equation for two particles not touching engaged in radiative heat exchange. Relative error between the two solutions is indicated by open symbols and is associated with the right vertical axis.

3.8 Closing Remarks

In this chapter, the various mechanisms of heat transfer present in gas-solids systems and the internal energy equation for a single, isothermal particle are defined. Subsequent sections review mathematical models for contact conduction, particle-fluid-particle conduction, particle-gas convection, and particle-particle radiation. For each of these mechanisms a specific model was chosen for implementation into an existing CFD-DEM code based on model simplicity, wide acceptance in existing CFD-DEM heat transfer models, extendibility to particles of different sizes, and computational expense.

Necessary modifications were made to selected models before implementing them into MFIX-DEM. Batchelor and O'Brien's [52] contact conduction model was generalized to compute the contact radius from the geometric configuration of the particles, and an effective thermal conductivity for the particles was defined (see Section 3.2.2). The particle-fluid-particle conduction model of Rong and Horio [16] was extended

to account for particles of different sizes (see Section 3.3.2). For particle-particle radiation, a new environment temperature was established (see Section 3.5.2).

Finally, the implementation of each model was verified for simple two particle test cases, or in the case of gas-particle convection, a single fixed particle in a flowing gas. Strong agreement was observed between the simulation data and the analytic or numerical solution.

Chapter 4: Particle-gas reactive chemistry interface

Chemical reactions in gas-solids flows may occur within a single phase (*homogeneous*) or they may require the presence of at least two phases (*heterogeneous*) [90]. Presently, MFIX, the CFD code portion of the CFD-DEM model employed in this work (MFIX-DEM), is capable of modeling user-defined homogeneous and heterogeneous chemical reactions among continuum phases (i.e., Eulerian-Eulerian models only) [91,92]. The goal of this effort is to develop and implement a mathematical interface for managing user-defined heterogeneous chemical reactions among the gas and discrete solids phases in MFIX-DEM.

This chapter begins by briefly defining the (1) reaction rate, (2) specific heat, (3) heat of reaction, and (4) individual particle mass and species equations in Section 4.1. Three particle reaction models and their employment in existing CFD-DEM reactive chemistry models are presented in Section 4.2. Finally, the algorithmic implementation and verification of the mathematical interface for managing user-defined particle-gas chemical reactions developed in this effort are given in Sections 4.3 and 4.4.

4.1 Foundations for particle-gas reactive chemistry

In this section, specific concepts of reactive chemistry referenced in this work are introduced. This is done to provide a foundation for the topics managed by the mathematical interface for user-defined chemical reactions. Additional details concerning the fundamentals of reactive chemistry are found in references [28,90,93,94].

4.1.1 Reaction rate

Various interrelated definitions for the rate at which a chemical reaction progresses, termed the *rate of reaction*, are available [90]. Therefore, care is needed to avoid ambiguity. This work defines the *rate of reaction with respect to species A* as the number of moles of species A formed (or consumed) per unit time, per unit surface area of a particle (e.g., $\text{mol}\cdot\text{cm}^{-2}\cdot\text{s}^{-1}$). Specifically, if species A is a *reactant*, then the rate of reaction is termed the *rate of disappearance of species A* and is notated as $-r_A$. Likewise, if species A is a *product* of the reaction, then the reaction rate is termed the *rate of formation of species A* and notated as r_A . The rate of disappearance is assigned a negative sign because the reaction rate is always specified as a non-negative number [93].

Defining the rate of reaction with respect to particle surface area is natural in the context of CFD-DEM as it allows for a 'per particle' treatment of particle-gas reactions. Other definitions (e.g., per volume of fluid or per reactor volume) may require averaging rates of formation and rates of disappearance of the solids phase species from a collection of particles contained within some control volume. This may, in effect, remove the distinct advantage of CFD-DEM modeling (i.e., the ability to track the conversion of individual particles during a chemical reaction).

The *rate equation* for a reaction (also referred to as a *rate law*) is an algebraic function which gives the reaction rate in terms of material properties [95]. An example rate law for the rate of formation of species A is shown in Equation (4-1). Here, k is the *rate coefficient* (also called the *rate constant*), C_A and C_B are the concentration of reactants A and B, and α and β are empirically fitted constants.

$$-r_A = kC_A^\alpha C_B^\beta \quad (4-1)$$

Once the rate of reaction with respect to a particular species is specified, the rates of formation and disappearance of the other reactants and products are obtained from the reaction stoichiometry. For example, consider the generic reaction shown in Equation (4-2). Here, a molecules of species A and b molecules of species B are destroyed to produce c molecules of species C and d molecules of species D. The terms in parentheses indicate whether the species belongs to the gas (g) or solids (s) phase. The proportional relationship linking the rates of disappearance of species A and B and the rates of formation of species C and D are given in Equation (4-3).

$$\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d} \quad (4-3)$$

Reactions where the reactants are consumed to form products, but the products do not react to form the reactants are termed *irreversible* and require a single reaction rate. The example reaction shown in Equation (4-2) is irreversible as indicated by the symbol ($\rightarrow$). However, rate equations are needed for both the *forward* and *backward* directions in *reversible* reactions, commonly indicated by the symbol ($\rightleftharpoons$). If the example reaction in Equation (4-2) were reversible, a reaction rate for the backward direction, potentially a function of the concentrations of species C and D, is needed.

4.1.2 Specific Heat

The amount of heat required to increase a material's temperature one degree, while holding the pressure or volume constant is termed the *heat capacity* [96]. The heat capacity at constant pressure is notated as C_p , and the heat capacity at constant volume is

notated C_p . The term *specific heat* is used to denote a heat capacity defined on a per unit mass basis. The specific heat of a material is a function of its temperature and commonly given as a polynomial [97]. Details concerning the calculation of specific heats in this effort are reserved for Section 4.3.3.

4.1.3 Heat of reaction

The amount of heat liberated or absorbed during a reaction, termed the *heat of reaction* (ΔH), is given by the difference in enthalpies between the products and reactants [90]. The change in enthalpy for *endothermic* reactions is positive, indicating that energy from the system is needed to facilitate the reaction. Conversely, the change in enthalpy for *exothermic* reactions is negative, signifying that energy is released to the system during the reaction. The heat of reaction for the generic reaction given by Equation (4-2) is illustrated by Equation (4-4). Here, H_C and H_D are the enthalpies of the products, and H_A and H_B are the enthalpies of the reactants.

$$\Delta H = (H_C + H_D) - (H_A + H_B) \quad (4-4)$$

The enthalpy for species n at temperature T ($H_n(T)$) is given by Equation (4-5). Here, $H_n^\circ(T_{REF})$ is species n 's *enthalpy of formation* at reference temperature T_{REF} , and ΔH_{Qn} is the enthalpy change caused by a change in temperature (i.e., from T_{REF} to T) [93]. The species change in enthalpy (ΔH_{Qn}) is calculated by integrating the material's specific heat (C_{pn}) with respect to temperature, as shown by Equation (4-6). Details concerning the calculation of enthalpies in this effort are reserved for Section 4.3.4.

$$H_n(T) = H_n^\circ(T_{REF}) + \Delta H_{Qn} \quad (4-5)$$

$$\Delta H_{Qn} = \int_{T_{REF}}^T C_{pn} dT \quad (4-6)$$

In reactions where mass is transferred from one phase to another (e.g., solids and gas phase species react to produce a different gas phase species), accounting for the transfer of enthalpy with the transferred mass is needed. Consider the example reaction shown in Equation (4-2). Suppose that there is a net production of gas phase species C and, in turn, a net consumption of solids phase species B (i.e., there is a net transfer of mass from the solids phase to the gas phase). The rate of enthalpy transfer as a result of mass transfer is then given by Equation (4-7). As before, $-r_B$ and r_D are the rate of disappearance and formation of solids species B and D, and H_C is the enthalpy of species C at the local gas phase conditions. If there are multiple destination phase products, care is needed to ensure that the rate of enthalpy transfer ($\dot{H}_{fr}$) is computed from the correct proportions and enthalpies of the various species generated.

$$\dot{H}_{fr} = H_C((-r_B) - r_D) \quad (4-7)$$

The usage of the transferred species' enthalpy at the destination phase's conditions is attributed to the *wet bulb effect* [98]. For example, as air passes over a wet wick covering a thermometer's bulb, some of the water evaporates. This causes the water's temperature to drop (i.e., the temperature reading on the thermometer drops). Once the temperature of the water stabilizes (i.e., there is a constant temperature reading from the thermometer), the heat loss from the water due to evaporation equals the heat gained by the water from the air. Otherwise, if energy from air was not transferred to the water, the water's temperature would continue to drop [99].

The heat of reaction and enthalpy transfer due to mass transfer are combined into source terms for the gas and particle internal energy equations (ΔH_{rg} in Equation (1-6) and ΔH_{sg} in Equation (3-6)). Since the heat of reaction is calculated for a reaction in general, a methodology for distributing the energy among the gas and solids phases is needed. The approach for assigning the heat of reaction employed in this effort is reserved for Section 4.3.5.

4.1.4 Mass and species equations for a particle

The time rate of change of a particle's mass resulting from a chemical reaction or phase change is given by Equation (4-8). Here, $m_p^{(i)}$ is the mass of the indexed particle, and $R_{sn}^{(i)}$ is the rate of production (or consumption) of species n for the indexed particle. The superscript over the summation, $N_s^{(i)}$, is the total number of species that comprise particle (i) . The sign convention is such that R_{sn} is positive if species n is produced and negative when consumed. Furthermore, R_{sn} is obtained from expressions like Equations (4-1) and (4-3) and specific to the reaction of interest.

$$\frac{dm_p^{(i)}}{dt} = \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \quad (4-8)$$

The time rate of change of the n^{th} species' mass in particle (i) is given by Equation (4-9). Here, $X_{pn}^{(i)}$ is species n 's mass fraction of the indexed particle. For a particle comprised by $N_s^{(i)}$ species, $N_s^{(i)}$ equations of this form are needed to account for the composition of the particle. Employing the *product rule* and combining the result with Equation (4-8) yields an equation for the species mass fraction, shown as (4-10).

$$\frac{d}{dt} (X_{pn}^{(i)} m_p^{(i)}) = R_{sn}^{(i)} \quad (4-9)$$

$$\frac{dX_{pn}^{(i)}}{dt} = \frac{1}{m_p^{(i)}} \left(R_{sn}^{(i)} - X_{pn}^{(i)} \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \right) \quad (4-10)$$

4.2 Particle reaction models

Three basic approaches for modeling the effect of a gas-solids reaction on a particle are surveyed in this section [90,100]. Various considerations needed to execute each model in MFIX-DEM are investigated. The result is that the unreacted-core model is best suited as the default particle reaction model for implementation into MFIX-DEM.

4.2.1 Progressive-conversion model

In highly porous particles, gaseous reactants may diffuse uniformly throughout a particle before reacting with the pores' surfaces [94]. This process, illustrated in Figure 4-1, is captured by the progressive-conversion model wherein the concentration of solids phase reactant diminishes evenly in the particle as a reaction proceeds.

Figure 4-1: Illustration of the progressive-conversion model. The reaction occurs uniformly throughout a particle, leaving the particle size unchanged. In this example, the concentration of the reactant diminishes as the reaction proceeds.

The assumption of constant particle volume applied to the particle mass equation (Equation (4-8)) provides an expression for the time rate of change of the particle's density, shown as Equation (4-11). The sign convention for the rate of solids phase

species production is such that a net production of solids mass causes the density of a particle to increase. Conversely, a net consumption of solids phase species results in a decrease of the particle's density.

$$\frac{d\rho_p^{(i)}}{dt} = \frac{1}{\mathcal{V}_p^{(i)}} \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \quad (4-11)$$

The progressive-conversion model is limited to slow reactions between a gas and very porous solid and reactions where a solid is converted exclusively by heat [90,94]. In the present effort, particles are assumed non-porous, and refining the particle model to include sub-particle pore structures is beyond the scope of this work. (More information on porous particle reaction models is found in reference [94].) Furthermore, physical experiments have shown that gas-solids reactions in non-porous solids typically progress from the particle's surface towards its center along a *reaction front* [90]. As a result, there is a separation of reacted and unreacted material within a particle, not a uniform conversion. Although the progressive-conversion model is implemented in the CFD-DEM code of Simsek et al. [22], it was not selected for this work in favor of a more physical approach.

4.2.2 Shrinking particle model

The shrinking particle model assumes the size of a particle decreases as a reaction proceeds. This is caused by an even gasification of the particle's components or a 'flaking-off' of solid products from the particle's surface. The shrinking particle model is illustrated in Figure 4-4 where the concentration of reactants in the particle remain constant as the particle's size decreases.

Figure 4-2: Illustration of the shrinking particle model. The reaction occurs at the particle's surface while the composition of the particle does not change. Any solid products of the reaction are assumed to 'flake off' of the particle's surface (i.e. no solid products collect on the surface of the particle).

By assuming the density of a particle is constant and that there are no solids phase products, the particle mass equation (Equation (4-8)) gives the time rate of change of the particle's radius, shown in Equation (4-12). The sign convention is such that the consumption of a particle's mass results in a decrease of the particle's radius. Since solids phase production is prohibited, R_{sn} is always non-positive.

$$\frac{dR_p^{(i)}}{dt} = \frac{1}{4\pi\rho_p^{(i)}R_p^{(i)2}} \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \quad (4-12)$$

The most notable limitation to the shrinking particle model is the opportunity for large disparities in particle sizes to develop (i.e., $R_p^{(i)} \ll R_p^{(j)}$). As the difference in particle sizes increase, the detection and storage of particle contact information may become computationally prohibitive. For example, in MFIX-DEM, each particle is the center of a *neighborhood*. Any particle whose center is contained within a particle's neighborhood is recorded as a potential contact partner. As the difference in particle sizes increase, the number of particles that are able to fit into a particle's neighborhood also increases. An exaggeration of how the computational expense could increase caused by an increase in size disparity among particles is illustrated Figure 4-3. A more robust

approach to contact detection and information storage is needed before this limitation is overcome.

Figure 4-3: An example illustrating how the number of possible neighbor particles increases as the ratio of the neighbor's radius (R_n) to the particle's radius (R_p) decreases.

This model additionally assumes that any solids phase products or inert material either gasify or ‘flake-off’ of a particle’s surface. This flaking-off of solids (ash) poses a difficult modeling task for CFD-DEM as discretizing and tracking any ash adds modeling complexity and computational expense. However, if the ash is not tracked (i.e., the ash is discarded or assumed negligible), then the conservation of solids mass is not maintained. Limiting simulations to those in which the initial particle contains no inert solids and all solids products are gasified is too restrictive for a general particle reaction model. Although the shrinking particle model is employed in several CFD-DEM reactive chemistry models [18,20,22,23,101], greater modeling flexibility is provided by a particle reaction model in which the production of solids phase species is permitted. As a result, the shrinking particle model is dismissed in favor of a more general approach.

4.2.3 Shrinking, unreacted-core model

In the shrinking, unreacted core model, a reaction starts on a particle’s surface and proceeds toward the particle’s center. As the reaction progresses, solids products from the reaction and any inert material initially in the particle form a continuous and even shell surrounding the unreacted core of the particle. Throughout the reaction, the unreacted

core shrinks uniformly while the thickness of inert solids (ash layer) increases uniformly. Illustrated in Figure 4-4, the outer radius of the particle and the concentration of reactants in the core remain constant as the core's radius decreases.

Figure 4-4: Illustration of the shrinking core model. The reaction occurs at the surface of the particle's unreacted core with an inert solid (ash) replacing the particle's solids. Although the unreacted core shrinks as the reaction proceeds, its composition remains constant.

Although not completely physical [90], the reaction front defines a sharp interface separating the ash layer from the unreacted core. An equation to specify the radial distance of the reaction front from the particle's center (R_c) is shown as Equation (4-13) where ρ_c is the density of the unreacted core, and $\hat{R}_{sn}$ is the rate of consumption of the solids phase reactants. This equation is obtained by considering only the reactants in the particle mass equation (i.e., Equation (4-8)).

$$\frac{dR_c^{(i)}}{dt} = \frac{-1}{4\pi\rho_c^{(i)}R_c^{(i)2}} \sum_{n=1}^{N_s^{(i)}} \hat{R}_{sn}^{(i)} \quad (4-13)$$

The definition of the unreacted core's density affects how its radius shrinks during the course of a reaction. For example, consider a particle-gas reaction where two solids phase species, B and C, are consumed. Furthermore, assume that there is an abundance of solid phase species C within the particle such that the excess species C remains in the particle after all the species B is consumed. The shrinking of the unreacted core employing three different definitions for the core's density is illustrated in Figure 4-5. In

the figure, the mass of species B and C (i.e., m_B and m_C) within the particle are indicated by the dashed and double lines. In this example, if the unreacted core's density (ρ_c) is equated to the particle's initial density (ρ_p), then the radius of the core shrinks to R_1 . If the unreacted core's density is defined as the bulk density of solids reactants initially in the particle, shown as Equation (4-14) where m_{sn}^0 is the initial mass of the solids phase reactant n and $\mathcal{V}_p$ is the particle's volume, then the radius of the core shrinks to R_2 . Finally, if the unreacted core's density is defined as the bulk density of consumable solids phase reactants, given by Equation (4-15) where m_{sn}^c is the total mass of solids phase reactant n consumed during the reaction, then the radius of the unreacted core shrinks to zero.

Figure 4-5: Example illustrating the connection between the radius of the unreacted core (R_c) and the definition of the unreacted core's density (R_c). If the unreacted core's density ($\rho_c = \rho_p$) is equated to the particle's initial density (ρ_p), then the core's radius shrinks to R_1 . If the unreacted core's density ($\rho_c = \rho_{\text{all reactants}}$) is defined as the initial mass of the solid phase reactants divided by the particle's volume, the core's radius shrinks to R_2 . Finally, if the unreacted core's density ($\rho_c = \rho_{\text{used reactants}}$) is defined as the total mass of solid phase reactants consumed divided by particle's volume, then the core's radius shrinks to zero.

$$\rho_c = \frac{1}{V_p} \sum_n m_{sn}^0 \quad (4-14)$$

$$\rho_c = \frac{1}{V_p} \sum_n m_{sn}^c \quad (4-15)$$

The above example leads to several observations. Note that if the initial composition of the particle is a single solids phase reactant, then all the definitions for the core density are the same. This is also true if there is no inert material initially present in the particle and the initial composition of the particle is balanced with the reaction stoichiometry (i.e., no solids phase reactants remain after the reaction is complete). However, if initially there is inert material in the particle and/or there is an abundance of one or more solids phase reactants, then the different solutions for the unreacted core's radius exist.

Additionally, the definitions for the unreacted core's density lead to several implicit assumptions. Consider the example illustrated in Figure 4-5. The unreacted core shrinks the least when the core's density is equated with the initial density of the particle. For this to occur, then the available solids reactants must exist in the outer region of the particle between R_1 and R_p . Similarly, the reactants must exist between R_2 and R_p when the unreacted core's density is given by Equation (4-14). By using Equation (4-15) to define the unreacted core's density, reactants are assumed uniformly distributed throughout a particle. This last definition also implies that any surplus solids reactants within a particle is treated as inert material.

Figure 4-6: Example illustrating the implicit assumptions associated with the definition of the unreacted core's density (R_c). If the unreacted core's density ($\rho_c = \rho_p$) is equated to the particle's initial density (ρ_p), then the consumable solids reactant exists between R_1 and R_p . If the unreacted core's density ($\rho_c = \rho_{\text{all reactants}}$) is defined as the initial mass of the solid phase reactants divided by the particle's volume, the consumable solids exist between R_2 and R_p . Finally, if the unreacted core's density ($\rho_c = \rho_{\text{used reactants}}$) is defined as the total mass of solid phase reactants consumed divided by particle's volume, then the consumable reactants are distributed uniformly through the particle.

The shrinking, unreacted core model was selected as the particle reaction model in this work. The selection was guided by (1) its near accurate physical account of particle-gas reactions [90], and (2) the ability to account for particles initially containing inert material. Although Liu, Chen, Zhou, and Zhao [21] claim to employ this model in their CFD-DEM, the authors cite a short simulation time (less than 15 seconds of physical time) to further assume that the diameter of the core is constant. This work makes no such assumption. The selection of the unreacted core's density is further addressed in Section 4.3.6. This concludes the survey of various particle reaction models. The following section outlines the implementation of the interface for managing particle-gas reactions into MFI-X-DEM.

4.3 Implementation of interface

The mathematical models managed in this effort by the reactive chemistry interface and discussed in the preceding sections, are summarized in Table 4-1. These models were implemented into MFI-X-DEM, an existing CFD-DEM code. This required the modification and creation of several subroutines. Descriptions of new subroutines are

outlined in Table 4-2, while the source code is reserved for Appendix E. Modifications to existing routines mainly consist of logical checks associated with call statements to the new routines. A call-tree showing the invocation of the reactive chemistry interface initialization routines is shown in Figure 4-7, and the invocation of the reactive chemistry interface model operational routines is shown by the call-tree in Figure 4-8.

Table 4-1: Summary of the models managed by the reactive chemistry interface considered in this work.

particle mass equation (Section 4.1.4)	$\frac{dm_p^{(i)}}{dt} = \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)}$
particle species mass fraction equation (Section 4.1.4)	$\frac{dX_{pn}^{(i)}}{dt} = \frac{1}{m_p^{(i)}} \left(R_{sn}^{(i)} - X_{pn}^{(i)} \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \right)$
particle internal energy equation (Section 3.1.3)	$m^{(i)} c_{pp}^{(i)} \frac{dT_p^{(i)}}{dt} = \dot{Q}_{pp}^{(i)} + \dot{Q}_{pfp}^{(i)} + \dot{Q}_{pg}^{(i)} + \dot{Q}_{rad}^{(i)} - \Delta H_{rs}^{(i)}$
shrinking, unreacted core radius (Section 4.2.3)	$\frac{dR_c^{(i)}}{dt} = \frac{-1}{4\pi\rho_c^{(i)} R_c^{(i)2}} \sum_{n=1}^{N_s^{(i)}} \hat{R}_{sn}^{(i)}$

Table 4-2: A list of subroutines developed for the reactive chemistry interface implemented into MFIX.

Subroutine <i>file name</i>	Description
DES_RXNS <i>des_rxns_mod.f</i>	Global data storage for common reaction data.
CHECK_DES_RXNS <i>check_des_rxns.f</i>	Checks the data provided for the reactive chemistry model, and sets various flags used to invoke the necessary subroutines.
DES_CALC_H <i>calc_h.f</i>	Calculates the enthalpy of the species using the current species temperature and the Burcat and Ruscic [102] thermodynamic database.
DES_PHYSICAL_PROP <i>des_physical_prop.f</i>	Calculates the temperature dependent specific heat of particles using the Burcat and Ruscic [102] thermodynamic database.
DES_RRATES <i>des_rrates.f</i>	Provides a set location within the code for a user to implement their specific reaction kinetics.
DES_REACTION_MODEL <i>des_reaction_model.f</i>	Update the mass, density, and species composition of the particles.

CALC_RRATES_DES <i>calc_rrates_des.f</i>	Invoke the DES_RRATES subroutine to calculate the interphase mass transfer and heat of reaction for the gas phase.
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Figure 4-7: Call graph of main MFIX-DEM source code for initialization routines. Dashed lines indicate new calls and subroutines implemented for the reactive chemistry interface.

Figure 4-8: Call graph of MFX discrete particle model routines. Dashed lines indicate new calls and subroutines implemented for the reactive chemistry interface.

A flow chart depicting the reactive chemistry interface implemented in MFX-DEM is presented in Figure 4-9. Processes added to the DEM algorithm for reactive chemistry are indicated by dashed lines.

Figure 4-9: Flow chart illustrating the locations within MFIx-DEM where modifications have been made to include the reactive chemistry interface.

4.3.1 Gas-solids mass and species mass transfer

The rates of disappearance and formation of gas and solids phases species, introduced in Section 4.1.1, result in an interphase coupling of the gas and particle mass balance equations as well as a coupling of the gas and particle mass balance species equations. Specifically, the rates of disappearance and formation of the gas and solids phase reactants and products result in source terms in the mass equations for the gas ($\sum_{n=1}^{N_g} R_{gn}$ in Equation (1-1)) and particle ($\sum_{n=1}^{N_s} R_{sn}$ in Equation (4-8)) as well as the species equations for the gas (R_{gn} in Equation (1-5)) and particle (R_{sn} in Equation (4-9)).

The approach used for interphase mass transfer follows directly from the method detailed in Section 3.6.1 for interphase energy transfer. Therefore, exchanging mass between the Eulerian grid and particles can occur through either a direct exchange between a particle and the Eulerian cell that contains its center, or through interpolating the information to the nearest Eulerian cells surrounding the particle (see Figure 3-24).

Equation (4-16) defines the species n mass production (or consumption), R_{gn} . Here, $\mathcal{V}_{CV}$ is the volume of the control volume (CV), N_{CV} is the number of particles contained in the CV, and $R_{gn}^{(k)}$ is the rate of gas phase species n production (or consumption) due to a particle-gas reaction between particle (k) and the gas phase. $K_{CV}^{(k)}$ is a function used to map the species mass to/from a particle's position from/to the computational nodes of the gas phase Eulerian grid.

$$R_{gn} = -\frac{1}{\mathcal{V}_{CV}} \sum_{k=1}^{N_{CV}} R_{gn}^{(k)} K_{CV}^{(k)} \quad (4-16)$$

As in the coupling of the gas and solids phase energy equations, there are two definitions for the mapping function, $K_{CV}^{(k)}$. By default, mass transfer between the gas and

a particle is associated with the CV containing the particle's center (see Figure 3-25-(a)). A second option distributes mass among the control volumes surrounding the particle via linear interpolation (see Figure 3-25-(b)). If the interpolation method is employed, the gas phase species concentrations, if needed by the rate law (see Equation (4-1) in Section 4.1.1), is interpolated to a particle's position from the surrounding control volumes for consistency.

The information (mass and species mass) exchanged between the gas and particles follows the same approach used for energy exchange. The source terms for the mass and species mass equations for the particles and gas are managed differently to account for the disjoint updating procedure (see Section 3.6.1). When the gas phase equations are solved, *all* of the physical properties of the particles are constant. This is a direct result of their solutions lagging behind the solution of the gas phase. Similarly, when the particle phase equations are solved, *all* of the physical properties of the gas phase are constant.

4.3.2 Mass, species mass, and core radius updating procedures

As mentioned in the updating procedure for the particle internal energy equation in Section 3.6.3, there are various methodologies available for solving differential equations numerically [87,88,89]. However, the time integration methods for the discrete solids phase momentum equation implemented in MFIX-DEM are limited to Euler's and Adams-Bashforth methods [35]. Therefore, the same methods are used to advance the solution for the particle's mass, species mass fraction, and core radius equations. Euler's method is the default approach selected by this work, and shown for the mass, species mass fraction, and unreacted core radius in Equations (4-17)-(4-19), respectively. Note

that both the mass and species mass fraction equations have a dependence on the particle's mass. Therefore, the particle's mass is updated first so that the new value for particle mass is available for updating the species mass fraction equations. The Adams-Bashforth method (not shown) is available for higher accuracy. Details concerning these methods are provided in references [88,89].

$$m_p^{(i)}(t + \Delta t_s) = m_p^{(i)}(t)\Delta t_s + \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \quad (4-17)$$

$$X_{pn}^{(i)}(t + \Delta t_s) = X_{pn}^{(i)}(t) + \frac{\Delta t_s}{m_p^{(i)}(t + \Delta t_s)} \left(R_{sn}^{(i)} - X_{pn}^{(i)} \sum_{n=1}^{N_s^{(i)}} R_{sn}^{(i)} \right) \quad (4-18)$$

$$R_c^{(i)}(t + \Delta t_s) = R_c^{(i)}(t) + \frac{-\Delta t_s}{4\pi\rho_c^{(i)} \left(R_c^{(i)}(t) \right)^2} \sum_{n=1}^{N_s^{(i)}} \hat{R}_{sn}^{(i)} \quad (4-19)$$

4.3.3 Specific heat calculations

Specific heat with respect to pressure, introduced in Section 4.1.2, indicates the amount of heat required to increase a material's temperature one degree per unit mass. The present work uses a fourth order polynomial to represent specific heat, as shown in Equation (4-20). The polynomial coefficients are obtained from the Burcat and Ruscic [102] thermodynamic database. Here, R is the gas constant, T is the temperature, and α_k are the polynomial coefficients obtained from the Burcat and Ruscic [102] database. Using this database, the specific heat is obtained in units of $\text{cal} \cdot (\text{mol} \cdot \text{K})^{-1}$.

$$C_{pn} = R \sum_{k=0}^4 \alpha_k T^k \quad (4-20)$$

The specific heat for a material composed of multiple species is approximated by combining the specific heats of the individual species weighted by their mass fraction. For example, the specific heat of a mixture composed of n species is illustrated in Equation (4-21). Here, T is the material temperature, and X is the species mass fraction of the indexed species.

$$C_p = \sum_{k=0}^4 \sum_{i=1}^n (\alpha_{ki} X_i) T^k \quad (4-21)$$

4.3.4 Heat of reaction calculations

The heat of reaction, ΔH , introduced in Section 3.4, specifies the amount of heat liberated or absorbed during a reaction [90]. Recall that the heat of reaction is calculated from the difference in enthalpies between the products and reactants. The enthalpy for a material at temperature T ($H_n(T)$) is obtained by combining the material's enthalpy of formation at reference temperature T_{REF} ($H_n^\circ(T_{REF})$) with the enthalpy change (ΔH_{Qn}) due to a change in temperature (T_{REF} to T) [93] (see Equation (4-5)). The change in enthalpy is calculated by integrating the specific heat with respect to temperature, (see Equation (4-6)). This work uses forth order polynomials for specific heat with the polynomial coefficients obtained from the Burcat and Ruscic [102] thermodynamic database (see Section 4.3.1). Integrating the generic polynomial structure results in an explicit expression for change in enthalpy, shown as Equation (4-22). Here, α_k are the polynomial coefficients, R is the gas constant, and T and T_{REF} are material and reference temperatures, respectively.

$$\Delta H_Q = \int_{T_{REF}}^T C_p dT = R \sum_{k=0}^4 \frac{\alpha_k}{(k+1)} (T^{k+1} - T_{REF}^{k+1}) \quad (4-22)$$

Similar to specific heat, the enthalpy for a material composed of multiple species is approximated by combining the enthalpies of the individual species weighted by their mass fraction. For example, the enthalpy of a mixture composed of n species is illustrated in Equation (4-23). Here, X is the mass fraction of the indexed species. The enthalpy of formation for species n at temperature T_{REF} divided by the gas constant ($H_i^\circ(T_{REF})/R$) is obtained from the Burcat and Ruscic [102] thermodynamic database with units of temperature (K).

$$H = R \left(\sum_{i=1}^n \left(\frac{H_i^\circ(T_{REF})}{R} \right) + \sum_{k=0}^4 \sum_{i=1}^n \left(\frac{\alpha_{ki}}{k+1} X_i \right) (T^{k+1} - T_{REF}^{k+1}) \right) \quad (4-23)$$

4.3.5 Distribution of the heat of reaction

The heat of reaction, ΔH , introduced in Section 3.4, is calculated in general for each reaction. A methodology for distributing the energy among the gas and solids phases is needed. The approach for assigning the heat of reaction employed in this effort is taken from Syamlal, Rogers, and O'Brien [27]. In their work, the heat of reaction associated with the gas phase is computed as the difference in enthalpies of the gas phase products and reactants. Similarly, the heat of reaction associated with the solids phase is computed as the difference in enthalpies of the solids phase products and reactants. Considering the example reaction given in Equation (4-2), the gas and solids phase heats of reaction are calculated by Equations (4-24) and (4-25), respectively.

$$\Delta H_g = H_C - H_A \quad (4-24)$$

$$\Delta H_s = H_D - H_B \quad (4-25)$$

The rate of heat production from the reaction is calculated by multiplying the enthalpies in the heat of reaction equations by their respective rates of formation or disappearance. The rates of energy production (or consumption) for the example reaction (see Equation (4-2)) associated with the gas and solids phases are given by Equations (4-26) and (4-27), respectively. Again, r_C and r_D are the rates of formation of species C and D, and r_A and r_B are the rates of disappearance of species A and B.

$$\Delta \dot{H}_g = H_C r_C - H_A (-r_A) \quad (4-26)$$

$$\Delta \dot{H}_s = H_D r_D - H_B (-r_B) \quad (4-27)$$

The heat of reaction for each phase and enthalpy transfer due to mass transfer (see Section 4.1.3 and Equation (4-7)) are combined into source terms for the gas and particle internal energy equations (ΔH_{rg} in Equation (1-6) and ΔH_{sg} in Equation (3-6)). Again, consider the example reaction shown in Equation (4-2). The net rate of heat generation for the gas phase is obtained by subtracting Equation (4-7) from Equation (4-26). The result, shown as Equation (4-28), is supplied to the internal energy equation for the gas phase (see Equation (1-6) in Section 1.1.1.4). Likewise, the net rate of heat generation for a particle is obtained by adding Equation (4-7) to Equation (4-27). The result, shown as Equation (4-29), goes into the particle internal energy equation. Note that the sign convention of the rate of enthalpy transfer ($\dot{H}_{fr}$) in Equations (4-28) and (4-29) depends on the direction of mass transfer (i.e., solids to gas, or gas to solids).

$$\Delta H_{rg} = \Delta \dot{H}_g - \dot{H}_{fr} \quad (4-28)$$

$$\Delta H_{rs} = \Delta \dot{H}_s + \dot{H}_{fr} \quad (4-29)$$

4.3.6 Unreacted core density

The radius in the shrinking, unreacted core model, introduced in Section 4.2.3, requires a closure model for the core's density. A general framework was created to provide easier customization of the reactive chemistry interface. This was achieved by providing a flag in the setup file (i.e., mfix.dat [84]) so that a user may define a specific core density. If the user does not specify the core density, it is equated to the particle's density by *default*. The generalization of the interface prevents Equations (4-14) and (4-15) from defining the default core density. Specifically, solids phase species are not explicitly identified as products or reactants within the code. Therefore, the amount of solids phase reactants (i.e., m_{sn}^0 in Equation (4-14) and m_{sn}^c in Equation (4-15)) is not calculable within the confines of the reactive chemistry interface's implementation.

4.4 Verification of implementation

Implementation of the reactive chemistry interface was verified using the case of a single reacting particle in a uniform gas flow. The gas-solid reaction is shown in Equation (4-30), where $A(g)$ and $B(s)$ are gas and solids phase reactants and $C(g)$ and $D(s)$ are gas and solids phase products. The particle initially contains solids reactant D, an inert solids phase material called I, and no solids product species D.

The reaction rate is given in terms of the rate of disappearance of species B, $(-r_B)$ and is assumed constant. The proportional relationship linking the rates of disappearance of species A and B and the rates of formation of species C and D are given in Equation (4-39). In this case the mass and species equations for the particle (see Equations (4-8)

and (4-9)) reduce to the expressions shown in Equations (4-32)-(4-35) describing the particle's mass and species mass fractions, respectively.

$$\frac{(-r_A)}{M_{sA}} = \frac{1}{2} \frac{(-r_B)}{M_{sB}} = \frac{r_C}{M_{sC}} = \frac{r_D}{M_{sD}} \quad (4-31)$$

$$\frac{dm_p}{dt} = (-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} - 1 \right) \quad (4-32)$$

$$\frac{d}{dt}(X_B m_p) = -(-r_B) \quad (4-33)$$

$$\frac{d}{dt}(X_D m_p) = \frac{1}{2} \frac{M_{sD}}{M_{sB}} (-r_B) \quad (4-34)$$

$$\frac{d}{dt}(X_I m_p) = 0 \quad (4-35)$$

Only heat transfer resulting from the reaction is considered (i.e., there is no convection, conduction, or radiation). In this case the internal energy equation describing the temperature of a particle (see Equation (3-6)) reduces to the expression shown in Equation (4-39). Here, m is the mass of the particle. C_{pp} , ΔH_s , and H_{fr} are defined in Equations (4-37)-(4-39) and represent the specific heat, change in enthalpy caused by the reaction, and the transfer of enthalpy due to mass transfer, respectively. In these equations, R is the gas constant, α_{ik} , $H_i^\circ(T_{REF})$, and M_{si} are the coefficients, reference enthalpies, and molecular weights of the indexed species obtained from the Burcat and Ruscic [102] thermodynamic database; X_i are the species mass fractions of the indexed species, and T_g and T_p are the gas phase and particle temperatures, respectively.

$$\frac{dT_p}{dt} = \frac{-1}{m_p C_{pp}} (\Delta \dot{H}_s + \dot{H}_{fr}) \quad (4-36)$$

$$\begin{aligned}\Delta\dot{H}_s = & (-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} H_D^\circ(T_{REF}) - H_B^\circ(T_{REF}) \right) \\ & + R \sum_{k=0}^4 \frac{(-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} \alpha_{Dk} - \alpha_{Bk} \right)}{(k+1)} (T_p^{k+1} - T_{REF}^{k+1})\end{aligned}\quad (4-37)$$

$$\dot{H}_{fr} = (-r_B) \left(1 - \frac{1}{2} \frac{M_{sD}}{M_{sB}} \right) \left(H_C^\circ(T_{REF}) + R \sum_{k=0}^4 \frac{\alpha_{Ck}}{(k+1)} (T_g^{k+1} - T_{REF}^{k+1}) \right) \quad (4-38)$$

$$C_{pp} = R \sum_{k=0}^4 \left(X_{pB} \frac{\alpha_{Bk}}{M_{sB}} + X_{pD} \frac{\alpha_{Dk}}{M_{sD}} + X_{pI} \frac{\alpha_{Ik}}{M_{sI}} \right) T_p^k \quad (4-39)$$

As before, analytic solutions for the particle's mass, species mass fractions, temperature, and unreacted core radius are obtained for a particle. All gas phase thermal and physical properties are assumed constant (C_{pg} and T_g). The particle's specific heat (C_{pp}) is assumed constant with respect to temperature. The density of the unreacted core is calculated from the bulk density of consumable solids phase reactants, given by Equation (4-15). These assumptions result in five ordinary differential equations solved by separation of variables. The resulting solutions for the particle's mass, species mass fractions, temperature, and unreacted core's radius are shown in Equations (3-34)-(3-39), respectively. Here, m_{p0} , X_{pB0} , X_{pD0} , X_{pI0} , and $T_{p,0}$ are the particle's initial mass, species mass fractions, and temperature, respectively.

$$m_p(t) = m_{p0} - t(-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} - 1 \right) \quad (4-40)$$

$$X_{pB}(t) = \frac{m_{p0} X_{pB0} - (-r_B) t}{m_{p0} - t(-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} - 1 \right)} \quad (4-41)$$

$$X_{pD}(t) = \frac{m_{p0}X_{pD0} + r_D t}{m_{p0} - t(-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} - 1 \right)} \quad (4-42)$$

$$X_{pI}(t) = \frac{m_{p0}X_{pI0}}{m_{p0} - t(-r_B) \left(\frac{1}{2} \frac{M_{sD}}{M_{sB}} - 1 \right)} \quad (4-43)$$

$$T_p(t) = \frac{1}{a_1} \left(\frac{b_2(a_1 T_{p0} + a_2)}{a_1 t + b_2} - a_2 \right) \quad \text{where}$$

$$a_1 = (-r_B) \frac{R}{M_{sB}} \left(\frac{\alpha_{D0}}{2} - \alpha_{B0} \right), \quad (4-44)$$

$$a_2 = (-r_B) R \left(\frac{1}{M_{sB}} \left(\frac{1}{2} \frac{H_D^\circ}{R} - \frac{H_B^\circ}{R} \right) + \frac{T_{REF}}{M_{sB}} \left(\alpha_{B0} - \frac{1}{2} \alpha_{D0} \right) + \frac{1}{M_{sC}} \left(1 - \frac{1}{2} \frac{M_{sD}}{M_{sB}} \right) \left(\frac{H_C^\circ}{R} \right) \right),$$

$$\text{and } b_2 = (m_{p0} R) \left(\frac{X_{B0} \alpha_{B0}}{M_{sB}} + \frac{X_{D0} \alpha_{D0}}{M_{sD}} + \frac{X_{I0} \alpha_{I0}}{M_{sI}} \right)$$

$$R_c = \left(R_p^3 - \frac{t(-r_B)}{\frac{4}{3} \pi \rho_c} \right)^{1/3} \quad (4-45)$$

A simulation employing the same assumptions as defined above was conducted with MFIX-DEM. The physical and thermodynamic properties of the particle, gas, and species components are outlined in Table 4-3 and Table 4-4. As the reaction is artificial, generic values were used for the thermodynamic properties and reaction rate. Realistic values are not necessary as this verification is designed to test the implementation of the various models, and not validate any specific chemical reaction. The simulation was run for 20 seconds of physical time to consume all of the available solids phase reactant (species B). The solids time step was kept constant at $\Delta t_s = 0.856357 \times 10^{-6}$. The simulation was performed on a single AMD Opteron 265, 1.8GHz processor.

Table 4-3: Physical and thermodynamic properties of the gas and particle used to verify the reactive chemistry interface implemented into MFIX-DEM.

particle diameter (cm)	0.30
Initial core diameter (cm)	0.30
Initial particle density (g/cm ³)	2.5
unreacted core density (g/cm ³)	1.25
Initial particle temperature (K)	500
gas temperature (K)	298
reaction rate: $(-r_B)$ (g of B consumed)	1.1781×10^{-3}
gas constant: R (cal/(mol·K))	1.98721
Reference Temperature: T_{REF} (K)	298

Table 4-4: Physical and thermodynamic properties of the gas and particle species used to verify the reactive chemistry interface implemented into MFIX-DEM.

Phase	Species	α_0	$H^\circ(T_{REF})/R$ (K)	M_s (g/mol)	Initial Mass Fraction
gas	A(g)	3.5	0	25	1.0
	C(g)	4.6	-1666.67	30	0.0
particle	B(s)	1.4	0	15	0.5
	D(s)	1.5	0	25	0.0
	I(s)	3	0	20	0.5

The numerical and analytical solutions for the particle's mass, species mass fraction, and temperature are shown in Figure 4-10, Figure 4-11, and Figure 4-12. Here, mp and Tp indicate the particle's mass and temperature; XB, XD, and XI represent the particle's species mass fractions, respectively. Solid symbols denote the values calculated by MFIX-DEM; continuous lines represent the analytic solution; and, open symbols indicate the error between the solutions. Percent relative error (see Equation (3-56)) is used in the analysis of the mass and energy equations. Absolute error, defined in Equation (4-46), was used in the analysis of the species mass fraction equations. Absolute error was needed because the analytic solution of species mass fraction for species B goes to zero, leading to a division by zero in Equation (3-56).

Note the strong agreement between the analytic and numeric solutions. The percent relative error for the mass and species equations is bounded above by 10^{-5} , indicating the numerical solution deviates less than $\pm 10^{-5}$ percent from the analytic solution over the entire simulation. The absolute error for the species mass fraction equations is bounded above by 10^{-6} , indicating an agreement between the solutions up to six decimal places over the entire simulation.

$$\text{Absolute Error} = \left| T_{pk}^{\text{analytic}} - T_{pk}^{\text{MFIx-DEM}} \right| \quad (4-46)$$

Figure 4-10: MFIx-DEM and analytic solutions to the particle mass equation engaged in reactive chemistry interface. mp is the mass of the particle. Relative error between the analytic and numeric (forward Euler method) solutions is indicated by open symbols and is associated with the right vertical axis.

Figure 4-11: MFIX-DEM and analytic solutions to the particle species equations engaged in reactive chemistry interface. XB, XD, and XI are the species mass fractions for species B, D, and I, respectively. Absolute error between the analytic and numeric (forward Euler method) solutions is indicated by open symbols and is associated with the right vertical axis.

Figure 4-12: MFIX-DEM and analytic solutions to the particle energy equation engaged in reactive chemistry interface. T_p is the temperature of the particle. Relative error between the analytic and numeric (forward Euler method) solutions is indicated by open symbols and is associated with the right vertical axis.

The numeric and analytic solutions for the radius of the unreacted core (R_c) is shown in Figure 4-13. Solid symbols denote the values calculated by MFIX-DEM; continuous line represents the analytic solution; and, open symbols indicate the error between the solutions. Absolute error (see Equation (4-46)) was used in the analysis because the analytic solution of core radius goes to zero. Note the strong agreement between the analytic and numerical solutions up to approximately 15 seconds wherein the absolute error is bounded above by 10^{-6} . However, the error is only bounded by $\pm 10^{-3}$ from this point forward. Neither forward Euler or Adams-Bashforth methods are able to capture the rapid decay of the unreacted core as the final amount of solids phase reactant (species B) is consumed. The reacting core's radius is not seen as a crucial modeling parameter. Therefore, a bounding of the absolute error from above by $\pm 10^{-3}$ is taken as acceptable for this effort.

Figure 4-13: MFIX-DEM and analytic solutions to the radius of the shrinking, unreacted core engaged in reactive chemistry interface. R_c is the core radius. Absolute error between the analytic and numerical (forward Euler and Adams-Bashforth (AB) methods) solutions are indicated by open symbols and is associated with the right vertical axis.

This verification shows a strong agreement between the analytic and numerical solutions for the mass, species mass fraction, and particle temperature equations. Similarly, agreement between analytic and numerical solutions for the shrinking, unreacted core is considered acceptable as it is a non-crucial modeling parameter. Therefore, the implementation of the reactive chemistry interface into the MFIX-DEM code is considered successful.

4.5 Closing Remarks

In this chapter, specific concepts of reactive chemistry referenced in this work was introduced. The subsequent section reviewed the mathematical models describing the effects of gas-solids reactions on a particle. The shrinking, unreacted core model (see Section 4.2.3) was selected for its relatively accurate physical account of particle-gas reactions and ability to account for particles initially containing inert material. Finally, the implementation of the reactive chemistry interface was verified for a single reacting particle. Strong agreement was observed between the simulation data and the analytic solution.

Chapter 5: Summary and recommendations

In this effort, MFI-X-DEM, an existing CFD-DEM, is enhanced to include discrete mass inflow-outflow boundary conditions (DMIBC or DMOBC), heat transfer, and an interface for managing user-defined chemical reactions. The following section provides a summary of these efforts. This chapter concludes by identifying several areas in which future work is offered to extend the functionality of the present effort.

5.1 Summary of results

5.1.1 Discrete mass boundary conditions

In Chapter 2, the algorithmic description of discrete mass inflow and outflow boundary conditions are presented. The inclusion of these functionalities allows models of more dynamic gas-solids systems by assigning user defined boundary conditions to the computational domain. An example wherein solids are fed into the bottom of a packed bed is given. This example illustrates the benefits of using a staging area outside of the computational domain. In doing so, new particles are fed into a system without disturbing the overall behavior of pre-existing particles. A second example is provided which overlaps a DMIBC and gas inflow boundary condition. This demonstrates how additional modeling flexibility is obtained through defining compound boundary conditions.

5.1.2 Particle heat transfer

Chapter 3 begins by defining the three modes of heat transfer and the internal energy equation for a single, isothermal particle. An examination of the assumption of isothermal particles is conducted which indicates that treating the particles as isothermal is appropriate. In the subsequent sections, an analysis of contact conduction, particle-

fluid-particle conduction, particle-gas convection, and particle-environment radiation are presented.

Batchelor and O'Brien's [52] model is selected as the foundation for developing a contact conduction model in this work. The selection is guided by the algebraic simplicity of the model, and wide employment of this model for particle-particle conduction in CFD-DEM [58,59,19,22,60,61]. Their model is extended in this work by defining an effective thermal conductivity between two particles. Additionally, Batchelor and O'Brien's [52] model is generalized by using the geometric configuration of touching particles to obtain the radius of their shared contact area. This results in a contact area representative of the specific collision model employed by the DEM (e.g., Cundall and Strack [44], Hertz [53], etc.), promoting greater modeling consistency throughout the CFD-DEM. The implementation of the particle-particle contact conduction model is verified for a simple two particle test case. Strong agreement is observed between the simulation data and the analytic solution.

Rong and Horio's [16] model is selected as the foundation for the particle-fluid-particle model developed in this work. This model is selected because of its relative simplicity, minimal computational expense, and extendibility to particles of different sizes. By establishing a standard point of reference, this model is additionally extended to particles of different size. The implementation of the particle-fluid-particle conduction model is verified by two simple test cases. In the first test case, two particles are close but not in contact, while in the second test, the particles are touching. Strong agreement is observed between the simulation data and the analytic solution for both test cases.

Particle-gas convection is assumed to follow Newton's law of cooling. Ranz and Marshall's [69] Nusselt number correlation is chosen to model the convective heat transfer coefficient. Their correlation is selected because of its employment in numerous CFD-DEM models [2,16,17,21,76]. Additionally, a general framework is created to facilitate implementation of additional correlations by users to provide greater customizability of the convective heat transfer model. This is achieved by providing a set location within the code for the user to implement their own correlation. The implementation of the particle-gas convection model is verified for a single fixed particle in a flowing gas. Strong agreement is observed between the simulation data and the analytic solution

A radiation model is developed based on an energy balance between two diffuse, gray surfaces [47]. The complexity of the model is reduced by assuming that neighboring particles form a spherical environment surrounding the particle of interest. An environmental temperature is established by averaging the temperature of the particles contained in a neighborhood surrounding the particle. Two limiting cases for the environment temperature produce definitions found in the literature [16,18,19,20]. The implementations of the radiative heat transfer model is verified for a simple two particle test case. Strong agreement is observed between the simulation data and a fourth order Runge-Kutta solution.

5.1.3 Particle-gas reactive chemistry interface

In Chapter 4, specific concepts of reactive chemistry referenced in this work are introduced. The shrinking, unreacted core model is selected as the particle reaction model for its relatively accurate physical account of particle-gas reactions and ability to account

for particles initially containing inert material. The implementation of the reactive chemistry interface is verified for a single reacting particle. Strong agreement is observed between simulation data and the analytic solutions for the particle's mass, species mass fraction, and internal energy equations. Agreement between the simulation data and analytic solution for the shrinking, unreacted core is considered acceptable.

5.2 Recommendations for future work

The discrete mass inflow and outflow boundaries provide significant flexibility to MFIX-DEM. Before this effort, a simulation started and ended with the same number of particles. With the inclusion of the discrete mass boundary conditions, the total amount of solids in a simulation is now permitted to fluctuate. However, there is a need for coupling the inflow/outflow boundaries so that as mass exits the system through the outlet, it reenters through the inlet. For example, the solids mass is constant in physical systems that employ a riser/standpipe combination. Solids exiting the riser are collected in the standpipe, then the solids in the standpipe are fed back into the riser. Therefore, the mass within the system is constant. In simulations of such physical systems, typically only the behavior within the riser is of interest. Computational expense is reduced by neglecting to model the standpipe. Constant solids mass within the simulation is enforced by directing out-flowing solids mass into a solids inlet (i.e., total solids flow out of the system equals the total solids flow into the system). *Therefore, this author recommends developing an additional discrete mass boundary condition such that out-flowing solids are re-introduced as inflow solids.*

System boundaries (walls) are assumed adiabatic (perfectly insulated) in this effort. As such, particle-wall heat transfer does not occur. This limitation is caused by the

approach employed in MFIX-DEM to detect particle-wall interactions. Presently, in MFIX-DEM, particle-wall interactions are managed *within* the collision model. By separating the particle-wall contact detection algorithm from the collision model this information is then available to other models. Specifically, the conduction and radiation models developed in this effort could manage particle-wall heat transfer if the interaction information is made available. *Therefore, this author suggests algorithmically restructuring where particle-wall detection is calculated in MFIX-DEM so that the information is available to all sub-models.*

The computational complexity of CFD-DEM restricts its applicability to small scale systems wherein there are few particles. Larger scale models are achievable by parallelizing CFD-DEM codes so that the computational burden is distributed among multiple processors. Currently, such efforts are undertaken for the hydrodynamic models in MFIX-DEM [103]. *To allow for large scale simulations with heat transfer and reactive chemistry, this author recommends including these sub-models in the current parallelization scheme.*

Finally, verification tests are conducted in this effort to ensure proper implementation of the selected/modified models. However, verification does not indicate whether the selected models accurately predict the physical behavior they represent. Three-dimensional (3-D) simulations containing a large number of particles are needed to generate data sets comparable with physical experiments. Presently, such simulations are not computationally tractable. However, larger scale simulations may become feasible once the heat transfer models and mathematical interface for particle scale reactions are parallelized. *Therefore, this author recommends conducting a model validation study*

once the models developed in this effort are incorporated into the current parallelization scheme.

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Appendix A: Geometric definitions for collision calculations

This section provides the geometric definitions for various terms needed for computing a two particle collision. A schematic of a collision is given in Figure A-1 to provide context for the various terms.

Figure A-1: Schematic demonstrating various terms needed in the calculation of the particle-particle collision force.

Consider the collision of two particles indexed by (i) and (j) where the particles' radii, positions, and linear and angular velocities are R_p , $\mathbf{X}$, $\mathbf{V}$, and $\boldsymbol{\omega}$, respectively. Then the following defines:

the normal overlap

$$\delta_n^{(i,j)} = R_p^{(i)} + R_p^{(j)} - \|\mathbf{X}^{(i)} - \mathbf{X}^{(j)}\|_2 \quad (\text{A-1})$$

unit normal from (i) to (j)

$$\boldsymbol{\xi}_n^{(i,j)} = \frac{\mathbf{X}^{(j)} - \mathbf{X}^{(i)}}{\|\mathbf{X}^{(j)} - \mathbf{X}^{(i)}\|_2} \quad (\text{A-2})$$

distance from center of particle (i) to the contact point

$$L^{(i)} = \frac{R_p^{(i)} - R_p^{(j)} + \|\mathbf{X}^{(j)} - \mathbf{X}^{(i)}\|_2}{2\|\mathbf{X}^{(j)} - \mathbf{X}^{(i)}\|_2} \quad (\text{A-3})$$

distance from center of particle (j) to the contact point

$$L^{(j)} = \|\mathbf{X}^{(j)} - \mathbf{X}^{(i)}\|_2 - L^{(i)} \quad (\text{A-4})$$

relative velocity of the point of contact

$$\mathbf{V}^{(i,j)} = \mathbf{V}^{(i)} - \mathbf{V}^{(j)} + \frac{1}{2}(L^{(i)}\boldsymbol{\omega}^{(i)} + L^{(j)}\boldsymbol{\omega}^{(j)}) \times \boldsymbol{\xi}_n^{(i,j)} \quad (\text{A-5})$$

normal relative velocity of the point of contact

$$\mathbf{V}_n^{(i,j)} = (\mathbf{V}^{(i,j)} \cdot \boldsymbol{\xi}_n^{(i,j)}) \boldsymbol{\xi}_n^{(i,j)} \quad (\text{A-6})$$

tangential relative velocity of the point of contact

$$\mathbf{V}_t^{(i,j)} = \mathbf{V}^{(i,j)} - \mathbf{V}_n^{(i,j)} \quad (\text{A-7})$$

unit tangential direction

$$\boldsymbol{\xi}_t^{(i,j)} = \frac{\mathbf{V}_t^{(i,j)}}{\|\mathbf{V}_t^{(i,j)}\|_2} \quad (\text{A-8})$$

tangential displacement at initial contact, t

$$\boldsymbol{\delta}_t^{(i,j)} = \mathbf{V}_t^{(i,j)} \min \left\{ \frac{|\delta_n|}{\mathbf{V}_t^{(i,j)} \boldsymbol{\xi}_n^{(i,j)}}, \Delta t_s \right\} \quad (\text{A-9})$$

tangential displacement at time $t + \Delta t$

$$\boldsymbol{\delta}_t^{(i,j)}(t + \Delta t) = \boldsymbol{\delta}_t(t) + \mathbf{V}_t^{(i,j)} \Delta t \quad (\text{A-10})$$

corrected tangential displacement at time $t + \Delta t$

$$\boldsymbol{\delta}_t^{(i,j)}(t + \Delta t) = \boldsymbol{\delta}_t^{(i,j)}(t + \Delta t) - \left(\boldsymbol{\delta}_t^{(i,j)}(t + \Delta t) \cdot \boldsymbol{\xi}_n^{(i,j)} \right) \boldsymbol{\xi}_n^{(i,j)} \quad (\text{A-11})$$

corrected unit vector in the tangential direction

$$\boldsymbol{\xi}_t' = \begin{cases} \boldsymbol{\xi}_t & \text{for } \boldsymbol{\xi}_t \neq \mathbf{0} \\ \frac{\boldsymbol{\delta}_t}{\|\boldsymbol{\delta}_t\|_2} & \text{for } \boldsymbol{\xi}_t = \mathbf{0}, \boldsymbol{\delta}_t \neq \mathbf{0} \end{cases} \quad (\text{A-12})$$

Additional details concerning these definitions are found in references [35,9].

Appendix B: Geometric definitions for conduction models

This section provides the geometric definitions for the contact radius and bounds of integration required by contact conduction and particle-fluid-particle conduction models. A schematic of the particles' geometric configuration is given in Figure A-1 to provide context for various terms.

B.1 Contact conduction definitions

Figure B-1: Schematic demonstrating various terms needed in the calculation of the contact radius needed for computing contact conduction. In this illustration particle i is smaller than particle j .

distance between particle centers

$$\ell^{(i,j)} = \|\mathbf{X}^{(i)} - \mathbf{X}^{(j)}\|_2 \quad (\text{B-1})$$

address the particle radii by the larger and smaller radii:

$$R^{(l)} = \min\{R^{(i)}, R^{(j)}\} \quad (\text{B-2})$$

$$R^{(k)} = \max\{R^{(i)}, R^{(j)}\} \quad (\text{B-3})$$

Figure B-2: Schematic demonstrating various terms needed in the calculation of the contact radius needed for computing contact conduction. In this illustration particle i is smaller than particle j .

law of Cosines:

$$R^{(l)^2} = R^{(k)^2} + \ell^{(k,l)^2} - 2 \ell^{(k,l)} R^{(k)} \cos \alpha \quad (\text{B-4})$$

$$\cos \alpha = \frac{R^{(k)^2} - R^{(l)^2} + \ell^{(k,l)^2}}{2 \ell^{(k,l)} R^{(k)}} \quad (\text{B-5})$$

Pythagorean theorem:

$$R_c^2 + \left(R_p^{(k)} \cos \alpha \right)^2 = R_p^{(k)^2} \quad (\text{B-6})$$

combining Equations (B-5) and (B-6) yields the contact radius:

$$R_c^2 + \left(R_p^{(k)} \frac{R^{(k)^2} - R^{(l)^2} + (\ell^{(k,l)})^2}{2 \ell^{(k,l)} R^{(k)}} \right)^2 = \left(R_p^{(k)} \right)^2 \quad (\text{B-7})$$

$$R_c^{(k,l)} = \sqrt{R^{(k)^2} - \left(\frac{R^{(k)^2} - R^{(l)^2} + \ell^{(k,l)^2}}{2 \ell^{(k,l)}} \right)^2} \quad (\text{B-8})$$

B.2 Particle-fluid-particle conduction definitions

Figure B-3: Schematic demonstrating various terms needed in the calculation of the contact radius needed for computing contact conduction. In this illustration particle i is smaller than particle j .

Abstracting to address the particle radii by the larger and smaller radii:

Figure B-4: Schematic demonstrating various terms needed in the calculation of the particle-fluid-particle conduction.

law of Cosines:

$$R^{(l)2} = (R^{(k)} + d^{(k)})^2 + \ell^{(k,l)2} - 2 \ell^{(k,l)} (R^{(k)} + d^{(k)}) \cos \alpha \quad (\text{B-9})$$

$$\cos \alpha = \frac{(R^{(k)} + d^{(k)})^2 - R^{(l)2} + \ell^{(k,l)2}}{2 \ell^{(k,l)} (R^{(k)} + d^{(k)})} \quad (\text{B-10})$$

Pythagorean theorem:

$$R_f^2 + ((R^{(k)} + d^{(k)}) \cos \alpha)^2 = (R^{(k)} + d^{(k)})^2 \quad (\text{B-11})$$

combining Equations (B-10) and (B-11) yields the outer region for particle-fluid-particle conduction:

$$R_f^2 + \left((R^{(k)} + d^{(k)}) \frac{(R^{(k)} + d^{(k)})^2 - R^{(l)2} + \ell^{(k,l)2}}{2 \ell^{(k,l)} (R^{(k)} + d^{(k)})} \right)^2 = (R^{(k)} + d^{(k)})^2 \quad (\text{B-12})$$

$$R_f^{(k,l)} = \sqrt{(R_p^{(k)} + d^{(k)})^2 - \left(\frac{(R_p^{(k)} + d^{(k)})^2 - R_p^{(l)2} + \ell^{(k,l)2}}{2 \ell^{(k,l)}} \right)^2} \quad (\text{B-13})$$

The section contains the source code for the discrete mass inflow and outflow boundary conditions. It has been written in the FORTRAN90/95 style.

```
! ~~~~~!  
! Module name: DES_INLET  
!  
! Purpose: Common elements needed for the des mass inflow boundary  
! condition.  
!  
! Author: J.Musser  
! Date: 13-Jul-09  
!  
! Comments:  
!  
! ^^^^^^^~  
  
MODULE DES_BC  
  
USE param  
  
! Logicals  
LOGICAL DES_MIO ! either inlet or outlet exists  
LOGICAL DES_MI ! inlet exists  
LOGICAL DES_MI_X, DES_MI_Y, DES_MI_Z ! inlet exists on IJK face  
LOGICAL DES_MO_X, DES_MO_Y, DES_MO_Z ! outlet exists on IJK face  
  
! Total DES mass inlets and outlets  
INTEGER DES_BCM_I ! inlet count  
INTEGER DES_BCM_O ! outlet count  
  
! Physical injection location  
DOUBLE PRECISION DES_BC_X_w(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_X_e(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_Y_s(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_Y_n(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_Z_b(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_Z_t(DIMENSION_BC)  
  
! Logical that indicates whether a boundary has been defined by the user  
LOGICAL DES_BC_DEFINED(DIMENSION_BC)  
  
! Specification for inflow into the system  
DOUBLE PRECISION DES_BC_VOLFLOW_s(DIMENSION_BC, DIM_M)  
DOUBLE PRECISION DES_BC_MASSFLOW_s(DIMENSION_BC, DIM_M)  
CHARACTER*16 DES_BC_TYPE(DIMENSION_BC)  
  
! DES mass inlet velocity at the BC plane  
DOUBLE PRECISION DES_BC_U_s(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_V_s(DIMENSION_BC)  
DOUBLE PRECISION DES_BC_W_s(DIMENSION_BC)  
  
! Macroscopic density of solids phases in a specified boundary region  
DOUBLE PRECISION DES_BC_ROP_s (DIMENSION_BC, DIM_M)  
  
! DES specification for solids phase velocity for WALL boundary  
! conditions. The current setup is fairly limited. The specified
```

```

! boundary velocities are assigned to the indicated wall where a wall
! corresponds to one of the six planes in a cubic domain. Each wall
! corresponds to a number as follows west=1, east=2, bottom=3, top=4,
! south=5, north=6. See cfwallposvel for details. To specify a y or z
! velocity to the west wall set des_bc_vw_s(1,M) or des_bc_ww_s(1,M),
! respectively (note an x velocity is not valid for a west or east wall).
! Since these are user input, they are allocated here with a constant
! preset size, but their actual size is represented by (nwalls, mmax)
      DOUBLE PRECISION DES_BC_Uw_s(DIMENSION_BC, DIM_M)
      DOUBLE PRECISION DES_BC_Vw_s(DIMENSION_BC, DIM_M)
      DOUBLE PRECISION DES_BC_Ww_s(DIMENSION_BC, DIM_M)

! Limit on the total number of divisions (fineness) used to represent
! the particle number distribution at an inlet.
      INTEGER, PARAMETER :: NUMFRAC_LIMIT = 10000

! Indicates if the boundary condition is mono or ploydisperse
! .F. = monodisperse and .T. = polydisperse
      LOGICAL, DIMENSION(:), ALLOCATABLE :: DES_BC_POLY      !(DES_BCMI)

! This array contains integers representing the mass/solid phase indices
! present at a specific boundary condition in proportion to their
! respective number fraction at the inlet (i.e., it represents the
! particle number distribution of incoming solids at the inlet). The
! array is scaled in size according to the parameter NUMFRAC_LIMIT.
      INTEGER, DIMENSION(:,:), ALLOCATABLE :: DES_BC_POLY_LAYOUT
!(DES_BCMI, NUMFRAC_LIMIT)

! DES boundary condition ID number (boundary number used in mfix.dat
! when the boundary is originally defined)
      INTEGER, DIMENSION(:), ALLOCATABLE :: DES_BC_MI_ID      !(DES_BCMI)
      INTEGER, DIMENSION(:), ALLOCATABLE :: DES_BC_MO_ID      !(DES_BCMO)

! Boundary classification
! Assigned a value of the face/edge associated with inlet in
! des_init_bc (see des_mi_classify)
! Possible values in 2D: 'YN', 'YS', 'XE', 'XW'
! Possible values in 3D: 'XZs', 'XZn', 'XYb', 'XYt', 'YZw', 'YZe'
      CHARACTER*3, DIMENSION(:), ALLOCATABLE :: DES_MI_CLASS    !(DES_BCMI)
! Assigned a value of the face/edge associated with outlet in
! des_init_bc (see des_mo_classify)
! Possible values in 2D: 'XW', 'XE', 'YN', 'YS'
! Possible values in 3D: 'XW', 'XE', 'YN', 'YS', 'ZB', 'ZT'
      CHARACTER*2, DIMENSION(:), ALLOCATABLE :: DES_MO_CLASS    !(DES_BCMO)
! Assigned a value in des_init_bc (see des_mi layout):
! When the inlet bc velocity is sufficiently high it is assigned
! 'RAND', otherwise it is assigned 'ORDR'
      CHARACTER*4, DIMENSION(:), ALLOCATABLE :: PARTICLE_PLCMNT
! Logical that can be flagged in the mfix.dat file to force the inlet
! to operate with an ordered boundary condition. This may be useful
! during long simulations or if the inlet appears to be taking a long
! time to randomly place particles.
      LOGICAL FORCE_ORD_BC

! Particle injection factor; how many solid time steps (dtsolid) pass
! before the next injection of a particle. if pi_count is greater than
! 1, then pi_factor is set to 1 (i.e. multiple particles enter every
! solids time step).
      INTEGER, DIMENSION(:), ALLOCATABLE :: PI_FACTOR      !(DES_BCMI)

! Particle injection count (injection number); how many particles are
! injected in one solids time step. pi_count is set to one if

```

```

! less than 1 particle enters per solids time step.
      INTEGER, DIMENSION(:), ALLOCATABLE :: PI_COUNT      !(DES_BCMI)

! Particle injection time scale; used when pi_factor > 1 to keep track
! of time needed for next injection
      DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DES_MI_TIME

! Order inlet condition variables: used when the variable
! particle_plcmnt is assigned 'ORDR'; in this case the inlet boundary is
! divided into grids and the particles are initially injected into an
! available grid cell
! -----
! keeps track of the number of grid cells that have been injected
! with a particle; is reset to 1 when all cells have been used.
      INTEGER, DIMENSION(:), ALLOCATABLE :: MI_FACTOR      !(DES_BCMI)
! the inlet edge/face is gridded and this variable stores the length
! dimension of the grid (no smaller than a particle diameter)
      DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: MI_WINDOW      !(DES_BCMI)
! Distance to offset incoming particles in ghost cells
      DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DES_BC_OFFSET      !(DES_BCMI)

! the dimension of this variable is equal to the number of grid
! cells in the inlet edge/face
      TYPE dmi
        INTEGER, DIMENSION(:), POINTER :: VALUE
      END TYPE dmi
! an array that stores integer values from 0 to a calculated factor in
! sequential order.
      TYPE(dmi), DIMENSION(:), ALLOCATABLE :: I_OF_MI
      TYPE(dmi), DIMENSION(:), ALLOCATABLE :: J_OF_MI      !(DES_BCMI)
! Construct an array of integers in values from 1 to a calculated factor
! in a random order, which is used when placing new particles.
      TYPE(dmi), DIMENSION(:), ALLOCATABLE :: MI_ORDER      !(DES_BCMI)
! -----

! Loop counter arrays: identifies the bounding i, j, k indices on the
! Eulerian/Continuum mesh (defined by imax, jmax, kmax) that encompasses
! an inlet boundary
      INTEGER, DIMENSION(:, :), ALLOCATABLE :: GS_ARRAY      !(DES_BCMI, 6)

END MODULE DES_BC

```

```

!-----
! Module name: CHECK_DES_BC
!-----
! Purpose: Check the data provided for the des mass inflow boundary
! condition and flag errors if the data is improper. This module is
! also used to convert the provided information into the format
! necessary for the dependent subroutines to function properly.
!-----
! Author: J.Musser                                Date: 13-Jul-09
!-----
! Comments:
!-----
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^

SUBROUTINE CHECK_DES_BC

    USE compar
    USE constant
    USE des_bc
    USE discretelement
    USE funits
    USE geometry
    USE indices
    USE param
    USE param1
    USE physprop
    USE run

    IMPLICIT NONE

!-----
! Local parameters
!-----
    INTEGER, PARAMETER :: DIM_BCTYPE = 4

!-----
! Local variables
!-----

! Loop counters
    INTEGER BCV, I
! Solids phase index
    INTEGER M
! tmp variable to calculate solids volume fraction at inlet
    DOUBLE PRECISION EPs_tmp
! valid boundary condition types
    CHARACTER*16, DIMENSION(1:DIM_BCTYPE) :: VALID_BC_TYPE = (/&
        'MASS_INFLOW      ', 'MI', '&
        'MASS_OUTFLOW     ', 'MO', '/')

!-----
! External functions
!-----
    LOGICAL , EXTERNAL :: COMPARE

!-----

! Initialize

```

```

DES_BCMI = 0; DES_MI = .FALSE.
DES_BCMO = 0
WRITE(*, '(3X,A)') '----- START CHECK_DES_BC ----->'

! Check for des inlet/outlet information:
CHECK_BC: DO BCV = 1, DIMENSION_BC
  DES_BC_DEFINED(BCV) = .FALSE.
  IF (DES_BC_X_w(BCV) /= UNDEFINED) DES_BC_DEFINED(BCV) = .TRUE.
  IF (DES_BC_X_e(BCV) /= UNDEFINED) DES_BC_DEFINED(BCV) = .TRUE.
  IF (DES_BC_Y_s(BCV) /= UNDEFINED) DES_BC_DEFINED(BCV) = .TRUE.
  IF (DES_BC_Y_n(BCV) /= UNDEFINED) DES_BC_DEFINED(BCV) = .TRUE.
  IF (DES_BC_Z_b(BCV) /= UNDEFINED) DES_BC_DEFINED(BCV) = .TRUE.
  IF (DES_BC_Z_t(BCV) /= UNDEFINED) DES_BC_DEFINED(BCV) = .TRUE.

! If a boundary location is specified, verify necessary data
  IF (DES_BC_DEFINED(BCV)) THEN
    IF (DES_BC_X_w(BCV) == UNDEFINED .OR. &
        DES_BC_X_e(BCV) == UNDEFINED .OR. &
        DES_BC_Y_s(BCV) == UNDEFINED .OR. &
        DES_BC_Y_n(BCV) == UNDEFINED) THEN
      WRITE (UNIT_LOG, 1000) BCV
      WRITE (*, 1000) BCV
      CALL MFIX_EXIT(myPE)
    ENDIF
    IF (DIMN == 3) THEN
      IF (DES_BC_Z_b(BCV) == UNDEFINED .OR. &
          DES_BC_Z_t(BCV) == UNDEFINED) THEN
        WRITE (UNIT_LOG, 1000) BCV
        WRITE (*, 1000) BCV
        CALL MFIX_EXIT(myPE)
      ENDIF
    ENDIF
    IF (DES_BC_X_w(BCV) .LT. ZERO .OR. &
        DES_BC_Y_s(BCV) .LT. ZERO .OR. &
        DES_BC_X_e(BCV) .GT. XLENGTH .OR. &
        DES_BC_Y_n(BCV) .GT. YLENGTH .OR. &
        DES_BC_X_w(BCV) .GT. DES_BC_X_e(BCV) .OR. &
        DES_BC_Y_s(BCV) .GT. DES_BC_Y_n(BCV)) THEN
      WRITE (UNIT_LOG, 1001) BCV
      WRITE (*, 1001) BCV
      CALL MFIX_EXIT(myPE)
    ENDIF
    IF (DIMN == 3) THEN
      IF (DES_BC_Z_b(BCV) .LT. 0 .OR. &
          DES_BC_Z_t(BCV) .GT. ZLENGTH .OR. &
          DES_BC_Z_b(BCV) .GT. DES_BC_Z_t(BCV)) THEN
        WRITE (UNIT_LOG, 1001) BCV
        WRITE (*, 1001) BCV
        CALL MFIX_EXIT(myPE)
      ENDIF
    ENDIF
  ENDIF

! Require the inlet/outlet to be on a boundary/wall of the system
  CALL DES_CHECK_MIO_LOCATION(BCV)

  DO I = 1, DIM_BCTYPE
    VALID_BC_TYPE(I) = TRIM(VALID_BC_TYPE(I))
    IF (VALID_BC_TYPE(I) == DES_BC_TYPE(BCV)) THEN
! If des_bc_type set with abbreviation form, then change to corresponding full
form
      IF (MOD(I,2) == 0) DES_BC_TYPE(BCV) = VALID_BC_TYPE(I-1)

```

```

! Check if solids phase velocity at the BC plane is specified, if not,
! set solids velocity to zero and flag log file
      IF (DES_BC_TYPE (BCV) == 'MASS_INFLOW') THEN
        DES_MI = .TRUE.
        DES_BCMI = DES_BCMI + 1

        Eps_tmp = ZERO
        DO M=1, MMAX
! If DES_BC_ROP_s is well defined (defined and not zero), check that either
! DES_BC_MASSFLOW or DES_BC_VOLFLOW is also well defined. If not, flag an
! error and exit.
          IF (DES_BC_ROP_s (BCV, M) /= UNDEFINED .AND. &
            .NOT. COMPARE (DES_BC_ROP_s (BCV, M), ZERO) ) THEN

! Check that density information is not missing, if so exit. RO_s is
! checked for unrealistic values in check_data_04.f
            IF (COMPARE (RO_s (M), ZERO) ) THEN
              WRITE (UNIT_LOG, 1006) M, BCV
              WRITE (*, 1006) M, BCV
              CALL MFIX_EXIT (myPE)
            ENDIF

! Check the values given for MASSFLOW and/or VOLFLOW
            IF (DES_BC_MASSFLOW_s (BCV, M) /= UNDEFINED) THEN
              IF (DES_BC_VOLFLOW_s (BCV, M) /= UNDEFINED) THEN
! Both volumetric and mass flow rates have been defined.
! Verify that the values match.
                IF (.NOT. COMPARE (DES_BC_VOLFLOW_s (BCV, M), &
                  DES_BC_MASSFLOW_s (BCV, M) / RO_s (M) ) ) THEN
                  WRITE (UNIT_LOG, 1006) BCV, M
                  WRITE (*, 1006) BCV, M
                  CALL MFIX_EXIT (myPE)
                ENDIF
              ELSE
! Only MASSFLOW was given. Calculate VOLFLOW.
                DES_BC_VOLFLOW_s (BCV, M) = &
                  DES_BC_MASSFLOW_s (BCV, M) / RO_s (M)
              ENDIF
            ELSE
! no mass flow rate is specified
              IF (DES_BC_VOLFLOW_s (BCV, M) == UNDEFINED) THEN
! If neither a volumetric or mass flow rate is specified, exit
                WRITE (UNIT_LOG, 1011) BCV, M
                WRITE (*, 1011) BCV, M
                CALL MFIX_EXIT (myPE)
              ENDIF
            ENDIF

! Add solids volume to total solids volume to check for overflow
            Eps_tmp = Eps_tmp + &
              (DES_BC_ROP_s (BCV, M) / RO_s (M) )
            ENDIF ! endif des_bc_rop_s is well defined

! Back check that if either DES_BC_MASSFLOW_s or DES_BC_VOLFLOW_s are
! well defined (defined and not zero), then ROP_s is also well defined.
            IF ((DES_BC_MASSFLOW_s (BCV, M) /= UNDEFINED .AND. &
              .NOT. COMPARE (DES_BC_MASSFLOW_s (BCV, M), ZERO) ) &
              .OR. &
              (DES_BC_VOLFLOW_s (BCV, M) /= UNDEFINED .AND. &
              .NOT. COMPARE (DES_BC_VOLFLOW_s (BCV, M), ZERO) ) ) THEN

              IF (DES_BC_ROP_s (BCV, M) == UNDEFINED .OR. &
                COMPARE (DES_BC_ROP_s (BCV, M), ZERO) ) THEN
! A nonzero mass or volumetric flow rate is defined for BCV on mass
! phase M, and either ROP_s is zero or undefined. Flag error and exit.

```

```

        WRITE(UNIT_LOG,1015)BCV,M
        WRITE(*,1015)BCV, M
        CALL MFIX_EXIT(myPE)
    ENDIF
ENDIF
ENDDO    ! end loop of M=1,MMAX

    IF(COMPARE(Eps_tmp,ZERO))THEN
! A des inlet has been defined, but there is no specifed flow information
! (no solids are entering)
        WRITE(UNIT_LOG,1013)BCV
        WRITE(*,1013)BCV
        CALL MFIX_EXIT(myPE)
    ELSEIF(Eps_tmp > ONE) THEN
! The total solids volume exceeds one
        WRITE(UNIT_LOG,1014)BCV
        WRITE(*,1014)BCV
        CALL MFIX_EXIT(myPE)
    ENDIF

    ELSE    ! if des_bc_type is not mass_inflow
        DES_BCMO = DES_BCMO + 1
    ENDIF    ! end if des_bc_type is MI, etc

! gives way to exit loop over des_bc_defined(bcv) when valid_bc_type is T
    CYCLE CHECK_BC

    ENDIF    ! endif des_bc_type is valid
ENDDO    ! end loop over dim_bc_type

! exit if des_bc_defined but bc_type is not valid
    WRITE (UNIT_LOG, 1002) BCV, DES_BC_TYPE(BCV)
    WRITE (*, 1002) BCV, DES_BC_TYPE(BCV)
    WRITE (UNIT_LOG, 1003) VALID_BC_TYPE
    WRITE (*, 1003) VALID_BC_TYPE
    WRITE (*, 1008)
    CALL MFIX_EXIT(myPE)

    ENDIF    ! end if des_bc_defined(bcv)

ENDDO CHECK_BC

WRITE(*,1012) DES_BCMO, DES_BCMO

IF(DES_BCMO /= 0 .OR. DES_BCMO /=0)THEN
    DES_MIO = .TRUE.
! Allocate necessary arrays for discrete mass inlets
    CALL ALLOCATE_DES_MIO(DES_BCMO, DES_BCMO)

! Verify that either the nsquare or grid based neighbor searches are
! used, otherwise flag and exit
    IF((DES_NEIGHBOR_SEARCH == 2) .OR. &
        (DES_NEIGHBOR_SEARCH == 3)) THEN
        WRITE (UNIT_LOG, 1005)
        WRITE (*, 1005)
        CALL MFIX_EXIT(myPE)
    ENDIF
ENDIF

! If the system is started without any particles and an inlet is not
! specified, the run is aborted.

```

```

IF(DES_BCMI == 0 .AND. PARTICLES == 0) THEN
  WRITE(UNIT_LOG, 1009)
  WRITE(*, 1009)
  CALL MFIX_EXIT(myPE)
ELSEIF(PARTICLES == 0) THEN
  WRITE(*, '(5X,A)') &
    'Run initiated with no particles in the system'
ENDIF

! Check MAX_PIS requirements
IF(DES_BCMI == 0 .AND. MAX_PIS == UNDEFINED_I) THEN
  WRITE(*, '(5X,A)') 'Setting MAX_PIS = PARTICLES'
  MAX_PIS = PARTICLES
ELSEIF(DES_BCMI /= 0 .AND. MAX_PIS == UNDEFINED_I) THEN
  WRITE(UNIT_LOG, 1010)
  WRITE(*, 1010)
  CALL MFIX_EXIT(myPE)
ENDIF

WRITE(*, '(3X,A)') '<----- END CHECK_DES_BC -----'

1000 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'Insufficient DEM boundary condition infomation',/10X,&
  'Check boundary condition number: ',I3,/1X,70('*')/)

1001 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Messsage: ',&
  'Improper DEM boundary condition information',/10X,&
  'Check boundary condition number: ',I3,/1X,70('*')/)

1002 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'Illegal BC_TYPE for boundary condition ',I3,/10X,&
  'BC_TYPE = ',A,' and the valid types are: ')
1003 FORMAT(5X,A16)

1004 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  A,' not specified in mfix.dat file for BC ',I3,/10X,&
  'Setting value to ZERO',/,1X,70('*')/)

1005 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'Currently, DEM inlet/outlet only supports the NSQUARE',/10X,&
  'and GRID_BASED_NEIGHBOR search methods.',/1X,70('*')/)

1006 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'Solids phase ',I3,' is used at DEM boundary condition ',I3,/10X,&
  'but its density RO_s is defined as zero.',/1X,70('*')/)

1007 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'Both DES_BC_MASSFLOW_s and DES_BC_VOLFLOW are defined',/10X,&
  'for boundary condition ',I3,' and solids phase ',I2,&
  ' but they',/10X, 'are not consistent.',/1X,70('*')/)

1008 FORMAT(/1X,70('*')/)

1009 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'The system is initiated with no particles and no DEM',/10X,&
  'inlet. The run is being terminated.',/1X,70('*')/)

1010 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
  'If a DEM inlet is specified then the maximum number of',/10X,&
  'particles permitted in the system (MAX_PIS) must be set',/10X,&

```



```

        'in mfix.dat',/1X,70('*')/)

1011 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
        'DES_BC_ROP_s is defined (and not zero) for boundary ',/10X,&
        'condition ',I3, ' and solids phase ',I2,' without defining',/10X,&
        'either DES_BC_MASSFLOW_s or DES_BC_VOLFOW.',/1X,70('*')/)

1012 FORMAT(5X,'No. of mass inlet BC = ', I4,/,&
        5X,'No. of mass outlet BC = ', I4)

1013 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
        'Boundary condition ',I3,' is identified as an DEM inlet',/10X,&
        'but has no associated inflow information. Check mfix.dat',&
        /1X,70('*')/)

1014 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
        'The total solids volume fraction for boundary condition',/10X,&
        I3,' exceeds one. Check the mfix.dat file.',/1X,70('*')/)

1015 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC',/, ' Message: ',&
        'A nonzero mass or volumetric flow rate has been specified',&
        'for',/10X,'boundary condition ', I3, ' and solids phase ',I3,/10X,&
        'and the associated DES_BC_ROP_s is either undefined or zero',/10X,&
        'Check mfix.dat',/,1X,70('*')/)

RETURN
END SUBROUTINE CHECK_DES_BC

```



```

        IF (DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
            DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV)) THEN
            WRITE (UNIT_LOG, 1101) &
            'For DIMN=2, DES mass inlet/outlet cannot be an area.', BCV
            WRITE (*, 1101) &
            'For DIMN=2, DES mass inlet/outlet cannot be an area.', BCV
            CALL MFIX_EXIT(myPE)
        ENDIF

    ELSE      ! if dimn != 2

        IF (DES_BC_X_w(BCV) == DES_BC_X_e(BCV)) THEN
            IF (DES_BC_X_w(BCV) /= ZERO .AND. DES_BC_X_w(BCV) /= XLENGTH) THEN
                IF (DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV)) THEN
! Require the inlet be a slit/edge on the XZ-face
                    IF (DES_BC_Y_s(BCV) /= ZERO .AND. &
                        DES_BC_Y_s(BCV) /= YLENGTH) THEN
                        WRITE (UNIT_LOG, 1100) BCV; WRITE (*, 1100) BCV
                        CALL MFIX_EXIT(myPE)
                    ENDIF
                ENDIF
                IF (DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV)) THEN
! Require the inlet be a slit/edge on the XY-face
                    IF (DES_BC_Z_b(BCV) /= ZERO .AND. &
                        DES_BC_Z_b(BCV) /= ZLENGTH) THEN
                        WRITE (UNIT_LOG, 1100) BCV; WRITE (*, 1100) BCV
                        CALL MFIX_EXIT(myPE)
                    ENDIF
                ENDIF
            ENDIF
! Require an area inlet to be on the YZ-face and the face must be at
! one of the x-boundary edges
            IF (DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV) .AND. &
                DES_BC_Z_b(BCV) /= DES_BC_Z_t(BCV)) THEN
                WRITE (UNIT_LOG, 1100) BCV; WRITE (*, 1100) BCV
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF
    ENDIF

    IF (DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV)) THEN
        IF (DES_BC_Y_s(BCV) /= ZERO .AND. DES_BC_Y_s(BCV) /= YLENGTH) THEN
            IF (DES_BC_X_w(BCV) == DES_BC_X_e(BCV)) THEN
! Require the inlet be a slit/edge on the YZ-face
                IF (DES_BC_X_w(BCV) /= ZERO .AND. &
                    DES_BC_X_w(BCV) /= XLENGTH) THEN
                    WRITE (UNIT_LOG, 1100) BCV; WRITE (*, 1100) BCV
                    CALL MFIX_EXIT(myPE)
                ENDIF
            ENDIF
            IF (DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV)) THEN
! Require the inlet be a slit/edge on the XY-face
                IF (DES_BC_Z_b(BCV) /= ZERO .AND. &
                    DES_BC_Z_b(BCV) /= ZLENGTH) THEN
                    WRITE (UNIT_LOG, 1100) BCV; WRITE (*, 1100) BCV
                    CALL MFIX_EXIT(myPE)
                ENDIF
            ENDIF
            IF (DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
                DES_BC_Z_b(BCV) /= DES_BC_Z_t(BCV)) THEN
! Require an area inlet to be on the XZ-face and the face must be at
! one of the y-boundary edges
                WRITE (UNIT_LOG, 1100) BCV; WRITE (*, 1100) BCV
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF
    ENDIF

```

```

        ENDIF
    ENDIF
ENDIF

    IF (DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV)) THEN
        IF (DES_BC_Z_b(BCV) /= ZERO .AND. DES_BC_Z_b(BCV) /= ZLENGTH) THEN
            IF (DES_BC_X_w(BCV) == DES_BC_X_e(BCV)) THEN
! Require the inlet be a slit/edge on the YZ-face
                IF (DES_BC_X_w(BCV) /= ZERO .AND. &
                    DES_BC_X_w(BCV) /= XLENGTH) THEN
                    WRITE (UNIT_LOG, 1100)BCV; WRITE (*, 1100)BCV
                    CALL MFIX_EXIT(myPE)
                ENDIF
            ENDIF
            IF (DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV)) THEN
! Require the inlet be a slit/edge on the XZ-face
                IF (DES_BC_Y_s(BCV) /= ZERO .AND. &
                    DES_BC_Y_s(BCV) /= YLENGTH) THEN
                    WRITE (UNIT_LOG, 1100)BCV; WRITE (*, 1100)BCV
                    CALL MFIX_EXIT(myPE)
                ENDIF
                IF (DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
                    DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV)) THEN
! Require an area inlet to be on the XY-face and the face must be at
! one of the z-boundary edges
                    WRITE (UNIT_LOG, 1100)BCV; WRITE (*, 1100)BCV
                    CALL MFIX_EXIT(myPE)
                ENDIF
            ENDIF
        ENDIF
    ENDIF

    ENDIF ! end if dimn == 2 / else

! The following checks target potential bc problems in 3D systems
! -----
    IF (DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
        DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV)) THEN
! Prohibit point-based mass inlet
        WRITE (UNIT_LOG, 1101)&
        'DES mass inlet/outlet must larger than a single point.',BCV
        WRITE (*, 1101)&
        'DES mass inlet/outlet must larger than a single point.',BCV
        CALL MFIX_EXIT(myPE)
    ENDIF
    IF (DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
        DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV) .AND. &
        DES_BC_Z_b(BCV) /= DES_BC_Z_t(BCV)) THEN
! Prohibit volume-based mass inlet
        WRITE (UNIT_LOG, 1101)&
        'For DIMN=3, DES mass inlet/outlet cannot be a volume.',BCV
        WRITE (*, 1101)&
        'For DIMN=3, DES mass inlet/outlet cannot be a volume.',BCV
        CALL MFIX_EXIT(myPE)
    ENDIF

    IF ((DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
        DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        ((DES_BC_X_w(BCV) == ZERO .AND. DES_BC_Y_s(BCV) == ZERO) &
        .OR. (DES_BC_X_w(BCV) == ZERO .AND. DES_BC_Y_s(BCV) == YLENGTH) &
        .OR. (DES_BC_X_w(BCV) == XLENGTH .AND. DES_BC_Y_s(BCV) == ZERO) &

```

```

        .OR. (DES_BC_X_w(BCV) == XLENGTH .AND. DES_BC_Y_s(BCV) == YLENGTH)))
.OR. &
    (DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
    DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
    ((DES_BC_X_w(BCV) == ZERO .AND. DES_BC_Z_b(BCV) == ZERO) &
    .OR. (DES_BC_X_w(BCV) == ZERO .AND. DES_BC_Z_b(BCV) == ZLENGTH) &
    .OR. (DES_BC_X_w(BCV) == XLENGTH .AND. DES_BC_Z_b(BCV) == ZERO) &
    .OR. (DES_BC_X_w(BCV) == XLENGTH .AND. DES_BC_Z_b(BCV) == ZLENGTH)))
.OR. &
    (DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
    DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
    ((DES_BC_Y_s(BCV) == ZERO .AND. DES_BC_Z_b(BCV) == ZERO) &
    .OR. (DES_BC_Y_s(BCV) == ZERO .AND. DES_BC_Z_b(BCV) == ZLENGTH) &
    .OR. (DES_BC_Y_s(BCV) == YLENGTH .AND. DES_BC_Z_b(BCV) == ZERO) &
    .OR. (DES_BC_Y_s(BCV) == YLENGTH .AND. DES_BC_Z_b(BCV) ==
ZLENGTH)))) THEN
! Prohibit DES mass inlet along domain edges
    WRITE (UNIT_LOG, 1101)&
    'DES mass inlet/outlet cannot be positioned in a corner.',BCV
    WRITE (*, 1101)&
    'DES mass inlet/outlet cannot be positioned in a corner.',BCV
    CALL MFIX_EXIT(myPE)
ENDIF

1100 FORMAT(/1X,70('*')//, ' From: DES_CHECK_MIO_LOCATION',/10X,&
    ' Message: DES boundary condition ',I4, ' must be ',/10X,&
    ' specified on a wall.',/1X,70('*'))

1101 FORMAT(/1X,70('*')//, ' From: DES_CHECK_MIO_LOCATION',/10X,&
    ' Message: ',A, /10X,'Check boundary condition ',I4,&
    ' in mfix.dat.',/1X,70('*'))

RETURN
END SUBROUTINE DES_CHECK_MIO_LOCATION

```

C.4 : Routine - ALLOCATE_DES_MIO

```
! ~~~~~!  
!  
! Module name: ALLOCATE_DES_MIO  
!  
! Purpose:  
!  
! Author: J.Musser  
! Date: 17-Aug-09  
!  
! Comments:  
!  
! ~~~~~!  
  
      SUBROUTINE ALLOCATE_DES_MIO  
  
      USE des_bc  
      USE discretelement  
  
      IMPLICIT NONE  
  
!-----  
! Local variables  
!-----  
      INTEGER I      ! Loop counter for no. of DES_BCMI  
  
!-----  
  
! Allocate/Initialize for inlets  
      IF(DES_BCMI /= 0) THEN  
  
! Boundary condition ID array  
      Allocate( DES_BC_MI_ID (DES_BCMI) )  
  
! Distance offset of incoming particles in ghost cell  
      Allocate( DES_BC_OFFSET (DES_BCMI) )  
  
! Particle injection factor  
      Allocate( PI_FACTOR (DES_BCMI) )  
  
! Particle injection count (injection number)  
      Allocate( PI_COUNT (DES_BCMI) )  
  
! Particle injection time scale  
      Allocate( DES_MI_TIME (DES_BCMI) )  
  
! Boundary classification  
      Allocate( DES_MI_CLASS (DES_BCMI) )  
      Allocate( PARTICLE_PLCMNT (DES_BCMI) )  
  
! Order inlet condition variables  
! (only needed if particle_plcmt is assigned 'ordr')  
      Allocate( MI_FACTOR (DES_BCMI) )  
      Allocate( MI_WINDOW (DES_BCMI) )  
      Allocate( MI_ORDER (DES_BCMI) )      ! type dmi  
      Allocate( I_OF_MI (DES_BCMI) )      ! type dmi  
      Allocate( J_OF_MI (DES_BCMI) )      ! type dmi  
  
! Grid search loop counter array; 6 = no. of faces  
      Allocate( GS_ARRAY (DES_BCMI, 6) )  
  
! Logical array stating if a bounday condition is polydisperse
```

```

        Allocate( DES_BC_POLY( DES_BCMI ) )

! Array used for polydisperse inlets: stores the particle number
! distribution of an inlet scaled with numfrac_limit
        Allocate( DES_BC_POLY_LAYOUT( DES_BCMI, NUMFRAC_LIMIT ) )

! Initialization
! Logical for whether inlet is polydisperse
        DES_BC_POLY(:) = .FALSE.
! Logical for inlet existence on IJK face
        DES_MI_X = .FALSE.
        DES_MI_Y = .FALSE.
        DES_MI_Z = .FALSE.
! Integer arrays
        DES_BC_MI_ID(:) = -1
        PI_FACTOR(:) = -1
        PI_COUNT(:) = -1
        MI_FACTOR(:) = -1
        MI_WINDOW(:) = -1
        GS_ARRAY(:, :) = -1
        DES_BC_POLY_LAYOUT(:, :) = -1
! Double precision arrays
        DES_MI_TIME(:) = UNDEFINED
! Character precision arrays
        DES_MI_CLASS(:) = UNDEFINED_C
        PARTICLE_PLCMNT(:) = UNDEFINED_C
! Derived data types
        DO I = 1, DES_BCMI
            NULLIFY( MI_ORDER(I)%VALUE )
            NULLIFY( I_OF_MI(I)%VALUE )
            NULLIFY( J_OF_MI(I)%VALUE )
        ENDDO

        ENDIF ! end if des_bcmi /= 0

! Allocate/Initialize for outlets
        IF(DES_BCMO /= 0) THEN

! Boundary Condition ID array
        Allocate( DES_BC_MO_ID (DES_BCMO) )

! Boundary classification
        Allocate( DES_MO_CLASS (DES_BCMO) )

! Initialization
! Integer arrays
        DES_BC_MO_ID(:) = -1
! Character arrays
        DES_MO_CLASS(:) = UNDEFINED_C
! Logical for outlet existence on IJK face
        DES_MO_X = .FALSE.
        DES_MO_Y = .FALSE.
        DES_MO_Z = .FALSE.

        ENDIF ! end if des_bcmo /= 0

        RETURN
    END SUBROUTINE ALLOCATE_DES_MIO

```

[illegible]

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(DESBCTYPE(BCV) == 'MASS_INFLOW')) THEN

    DESBCMIID(BCV_I) = BCV

! Initialize temp variables
!   The number of mass phases at this inlet. While a system may be
!   polydisperse, the inlet could consist of a single mass phase
    PHASECNT = 0
!   The mass phase indices of incoming particles at this inlet
    PHASELIST(:) = -1
!   The max diameter of incoming particles at this inlet
    MAXDIA = ZERO

! Determine if the inlet is mono or polydisperse
    DO M=1, MMAX
        IF (DESBCTOP_s(BCV,M) /= UNDEFINED .AND. &
            .NOT.COMPARE(DESBCTOP_s(BCV,M),ZERO)) THEN
            PHASECNT = PHASECNT + 1
            PHASELIST(PHASECNT) = M
            MAXDIA = MAX(MAXDIA,DPO(M))
        ENDIF
    ENDDO

! Flag that the inlet is polydisperse if true
    IF(PHASECNT > 1) DESBCPOLY(BCV_I) = .TRUE.

! Set the value of the boundary condition offset value used in the
! placement of new particles.
    DESBCOFFSET(BCV_I) = MAXDIA

! Initialize temp variables
!   Number of phase m particles at BCV injected per second
    NPMpSEC(:) = ZERO
!   Total number of particles at BCV injected per second
    NPpSEC = ZERO
!   Total number of particles injected per solids time step
    NPpDT = ZERO

! calculate the number of particles of mass phase M are injected per
! second for each solid phase present at the boundary
    DO MM=1, PHASECNT
        M = PHASELIST(MM)
        NPMpSEC(M) = (DESBCTOP_s(BCV,M) / &
            (PI/6.d0 * DPO(M)**3))
        WRITE(*,"(5X,A,I2,A,F9.5)") &
            'NPMpSEC(',M,'): ',NPMpSEC(M)
! calculate the total number of particles per second at the inlet
        NPpSEC = NPpSEC + NPMpSEC(M)
    ENDDO

    WRITE(*,"(5X,A,F12.6)") 'NPpSEC: ',NPpSEC

! For polydisperse inlets, construct the DESPOLY_LAYOUT array
    IF(DESBCTOP_s(BCV_I)) THEN
!
        HOLD = 1
        RANGEBOT = 1
        DO MM=1, PHASECNT - 1
            M = PHASELIST(MM)
            SCALED_VAL = dble(NUMFRAC_LIMIT) * (NPMpSEC(M) / NPpSEC)
            RANGETOP = FLOOR(SCALED_VAL) + (RANGEBOT-1)
!
            DO I=HOLD, FLOOR(SCALED_VAL) + (HOLD-1)
!
                DESPOLY_LAYOUT(BCV_I,I) = M
!
            ENDDO
        ENDDO
    ENDIF

```

```

        DES_BC_POLY_LAYOUT(BCV_I,RANGE_BOT:RANGE_TOP) = M
        RANGE_BOT = RANGE_TOP+1
!
        HOLD = I
    ENDDO
    M = PHASE_LIST(PHASE_CNT)
!
    DO I=HOLD,NUMFRAC_LIMIT
!
        DES_POLY_LAYOUT(BCV_I,I) = M
!
    ENDDO
    DES_BC_POLY_LAYOUT(BCV_I,RANGE_BOT:NUMFRAC_LIMIT) = M
! For monodisperse inlets, store the single mass phase used
    ELSE
        DES_BC_POLY_LAYOUT(BCV_I,:) = PHASE_LIST(1)
    ENDIF

! The number of total particles per solid time step DTSOLID
    NPpDT = NPpSEC * DTSOLID

    IF(NPpDT .LT. 1)THEN
! The number of solid time steps between injection of a particle
        PI_FACTOR(BCV_I) = FLOOR(real(1.d0/NPpDT))
        PI_COUNT(BCV_I) = 1
    ELSE
        PI_FACTOR(BCV_I) = 1
! The number of particles injected in a solid time step
        PI_COUNT(BCV_I) = CEILING(real(NPpDT))
    ENDIF

    WRITE(*,"(5X,A,F12.6)") 'NPpDT: ',NPpDT

! Calculate des mass inlet time; time between injection. If the run
! type is RESTART_1, DES_MI_TIME will be picked up from the restart file
! with an updated value.
    IF(RUN_TYPE == 'NEW')THEN
        DES_MI_TIME(BCV_I) = TIME +&
            dble(PI_FACTOR(BCV_I)) * DTSOLID
    ENDIF
    WRITE(*,1000) BCV, NPpDT, PI_FACTOR(BCV_I),&
        PI_COUNT(BCV_I), DES_MI_TIME(BCV_I)

! Classify boundary condition and verify appropriate solids velocity
    CALL DES_MI_CLASSIFY(BCV, BCV_I, MAX_DIA, PHASE_CNT,&
        PHASE_LIST)

! Determine the computational cells near the inlet
    CALL DES_MI_CELLS(BCV, BCV_I)

! Verify that the inlet is not 'too' close to a periodic boundary condition
    IF(DES_PERIODIC_WALLS)THEN
        CALL DES_MIO_PERIODIC(BCV, BCV_I,'MI',MAX_DIA)
    ENDIF

    BCV_I = BCV_I + 1
    ENDIF
    ENDDO
ENDIF

! Check each discrete mass outlet for necessary data
    IF(DES_BCMO/=0)THEN
        BCV_I = 1
        DO BCV = 1, DIMENSION_BC
            IF((DES_BC_DEFINED(BCV)) .AND. &
                (DES_BC_TYPE(BCV) == 'MASS_OUTFLOW'))THEN

```

```

        DES_BC_MO_ID(BCV_I) = BCV

        CALL DES_MO_CLASSIFY(BCV_I, BCV)

! Verify that the outlet is not too close to a periodic boundary condition
        IF(DES_PERIODIC_WALLS) THEN
            CALL DES_MIO_PERIODIC(BCV,BCV_I,'MO',MAX_DIA)
        ENDIF

        BCV_I = BCV_I + 1
    ENDIF
ENDDO
ENDIF

WRITE(*,'(3X,A)') '<----- END DES_INIT_BC -----'

1000 FORMAT(/5X,'For mass inlet BC: ', I3,/, &
    7X,'No. particles injected per solids time step = ', ES15.8,/, &
    7X,'PI_FACTOR = ', I, ' PI_COUNT = ', I5,/, &
    7X,'start DES_MI_TIME = ', ES15.8)

RETURN
END SUBROUTINE DES_INIT_BC

```

```

! ~~~~~!
! Module name: DES_MI_CLASSIFY!
!
! Purpose: This subroutine is used to give a classification to the!
! inlet. The classification is used in the placement of new particles!
! in ghost cells behind the inlet.!
!
! Author: J.Musser!
! Date: 14-Aug-09!
!
! Comments:
!
! ~~~~~!

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ENDIF

! Check horizontal mass inlet: 2D
! -----
      IF (DES_BC_Y_s (BCV) == DES_BC_Y_n (BCV)) THEN

! Classify the boundary condition
      IF (DES_BC_Y_s (BCV) == ZERO) DES_MI_CLASS (BCV_I) = 'YS'
      IF (DES_BC_Y_s (BCV) == YLENGTH) DES_MI_CLASS (BCV_I) = 'YN'

! Inlet length
      LEN1 = DES_BC_X_e (BCV) - DES_BC_X_w (BCV)
ENDIF

! max_dia is used for the 'depth/width' of the inlet
! (see des_bc_vel_assign for details)
      CALL DES_BC_VEL_ASSIGN (BCV, BCV_I, LEN1, MAX_DIA, PHASE_CNT, PHASE_LIST)

! This subroutine determines the pattern that the particles will need to
! enter the system, if any. This routine only needs to be called if a
! run is new. If a run is a RESTART_1, all of the setup information
! provided by this subroutine is will be obtained from the *_DES.RES file.
! This is done due to this routine's strong dependence on the
! RANDOM_NUMBER() subroutine.
      IF (RUN_TYPE == 'NEW') THEN
        CALL DES_MI_LAYOUT (LEN1, ZERO, BCV, BCV_I, MAX_DIA, &
          PHASE_CNT, PHASE_LIST)
      ENDIF

      ELSE ! 3D domain

! Check mass inlet on XZ face: 3D
! -----
! see comments following the yz face section for elucidation on this
! series of if statements
      IF (DES_BC_Y_s (BCV) == DES_BC_Y_n (BCV) .AND. &
        DES_BC_X_w (BCV) /= DES_BC_X_e (BCV) .AND. &
        DES_BC_Z_b (BCV) /= DES_BC_Z_t (BCV) &
        .OR. &
        DES_BC_Y_s (BCV) == DES_BC_Y_n (BCV) .AND. &
        DES_BC_X_w (BCV) == DES_BC_X_e (BCV) .AND. &
        DES_BC_X_w (BCV) /= ZERO .AND. &
        DES_BC_X_w (BCV) /= XLENGTH &
        .OR. &
        DES_BC_Y_s (BCV) == DES_BC_Y_n (BCV) .AND. &
        DES_BC_Z_b (BCV) == DES_BC_Z_t (BCV) .AND. &
        DES_BC_Z_b (BCV) /= ZERO .AND. &
        DES_BC_Z_b (BCV) /= ZLENGTH) THEN

! If a slit flow inlet is specified near an edge, expand the slit to
! the width of one particle diameter :
! see comments in the yz face section for further explanation
      IF (DES_BC_X_w (BCV) == DES_BC_X_e (BCV)) THEN
        IF (((DES_BC_X_w (BCV) - MAX_DIA*HALF) .GE. ZERO) .AND. &
          ((DES_BC_X_w (BCV) + MAX_DIA*HALF) .LE. XLENGTH)) THEN
          DES_BC_X_w (BCV) = DES_BC_X_w (BCV) - MAX_DIA*HALF
          DES_BC_X_e (BCV) = DES_BC_X_e (BCV) + MAX_DIA*HALF
        ELSEIF ((DES_BC_X_w (BCV) - MAX_DIA*HALF) .LT. ZERO) THEN
          DES_BC_X_w (BCV) = ZERO
          DES_BC_X_e (BCV) = MAX_DIA
        ELSEIF ((DES_BC_X_e (BCV) + MAX_DIA*HALF) .GT. XLENGTH) THEN
          DES_BC_X_w (BCV) = XLENGTH - MAX_DIA

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        DES_BC_X_e(BCV) = XLENGTH
    ENDIF
ENDIF
IF(DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV)) THEN
    IF(((DES_BC_Z_b(BCV) - MAX_DIA*HALF) .GE. ZERO) .AND. &
        ((DES_BC_Z_b(BCV) + MAX_DIA*HALF) .LE. ZLENGTH)) THEN
        DES_BC_Z_b(BCV) = DES_BC_Z_b(BCV) - MAX_DIA*HALF
        DES_BC_Z_t(BCV) = DES_BC_Z_t(BCV) + MAX_DIA*HALF
    ELSEIF((DES_BC_Z_b(BCV) - MAX_DIA*HALF) .LT. ZERO) THEN
        DES_BC_Z_b(BCV) = ZERO
        DES_BC_Z_t(BCV) = MAX_DIA
    ELSEIF((DES_BC_Z_t(BCV) + MAX_DIA*HALF) .GT. ZLENGTH) THEN
        DES_BC_Z_b(BCV) = ZLENGTH - MAX_DIA
        DES_BC_Z_t(BCV) = ZLENGTH
    ENDIF
ENDIF
ENDIF

! Classify the boundary condition
IF(DES_BC_Y_s(BCV) == ZERO) DES_MI_CLASS(BCV_I) = 'Xzs'
IF(DES_BC_Y_s(BCV) == YLENGTH) DES_MI_CLASS(BCV_I) = 'Xzn'

! Inlet dimensions
LEN1 = DES_BC_X_e(BCV) - DES_BC_X_w(BCV)
LEN2 = DES_BC_Z_t(BCV) - DES_BC_Z_b(BCV)

ENDIF ! End check mass inlet on XZ face: 3D

! Check mass inlet on XY face: 3D
! -----
! see comments following the yz face section for elucidation on this
! series of if statements
IF(DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
    DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
    DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV) &
    .OR. &
    DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
    DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
    DES_BC_X_w(BCV) /= ZERO .AND. &
    DES_BC_X_w(BCV) /= XLENGTH &
    .OR. &
    DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
    DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
    DES_BC_Y_s(BCV) /= ZERO .AND. &
    DES_BC_Y_s(BCV) /= YLENGTH) THEN

! If a slit flow inlet is specified near an edge, expand the slit to
! the width of one particle diameter :
! see comments in the yz face section for further explanation
IF(DES_BC_X_w(BCV) == DES_BC_X_e(BCV)) THEN
    IF(((DES_BC_X_w(BCV) - MAX_DIA*HALF) .GE. ZERO) .AND. &
        ((DES_BC_X_w(BCV) + MAX_DIA*HALF) .LE. XLENGTH)) THEN
        DES_BC_X_w(BCV) = DES_BC_X_w(BCV) - MAX_DIA*HALF
        DES_BC_X_e(BCV) = DES_BC_X_e(BCV) + MAX_DIA*HALF
    ELSEIF((DES_BC_X_w(BCV) - MAX_DIA*HALF) .LT. ZERO) THEN
        DES_BC_X_w(BCV) = ZERO
        DES_BC_X_e(BCV) = MAX_DIA
    ELSEIF((DES_BC_X_e(BCV) + MAX_DIA*HALF) .GT. XLENGTH) THEN
        DES_BC_X_w(BCV) = XLENGTH - MAX_DIA
        DES_BC_X_e(BCV) = XLENGTH
    ENDIF
ENDIF
ENDIF
IF(DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV)) THEN
    IF(((DES_BC_Y_s(BCV) - MAX_DIA*HALF) .GE. ZERO) .AND. &

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        ((DES_BC_Y_s(BCV) + MAX_DIA*HALF) .LE. YLENGTH)) THEN
        DES_BC_Y_s(BCV) = DES_BC_Y_s(BCV) - MAX_DIA*HALF
        DES_BC_Y_n(BCV) = DES_BC_Y_n(BCV) + MAX_DIA*HALF
    ELSEIF((DES_BC_Y_s(BCV) - MAX_DIA*HALF) .LT. ZERO) THEN
        DES_BC_Y_s(BCV) = ZERO
        DES_BC_Y_n(BCV) = MAX_DIA
    ELSEIF((DES_BC_Y_n(BCV) + MAX_DIA*HALF) .GT. YLENGTH) THEN
        DES_BC_Y_s(BCV) = YLENGTH - MAX_DIA
        DES_BC_Y_n(BCV) = YLENGTH
    ENDIF
ENDIF

! Classify the boundary condition
IF(DES_BC_Z_b(BCV) == ZERO) DES_MI_CLASS(BCV_I) = 'XYb'
IF(DES_BC_Z_b(BCV) == ZLENGTH) DES_MI_CLASS(BCV_I) = 'XYt'

! Inlet dimensions
LEN1 = (DES_BC_X_e(BCV) - DES_BC_X_w(BCV))
LEN2 = (DES_BC_Y_n(BCV) - DES_BC_Y_s(BCV))

ENDIF ! End check mass inlet on XY face: 3D

! Check mass inlet on YZ face: 3D
! -----
! from previous checks in des_check_mio_location the combination of xe==xw,
! yn==ys, ys!=zero and ys!=ylength implies two items:
!   that xw is either zero or xlength, since if xw was zero or xlength then
!     ys could not be zero or ylength (or the boundary would be on the
!     domain edge which is prohibited)
!   that zt!=zb, since zt==zb would result in a prohibited point boundary
! similarly the combination of xe==xw, zt==zb, zb!=zero and zb!=zlength
! implies the following:
!   that xw is either zero or xlength, since if xw was zero or xlength then
!     zb could not be zero or zlength (or the boundary would be on the
!     domain edge which is prohibited)
!   that yn!=ys, since yn==ys would result in a prohibited point boundary
IF(DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
   DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV) .AND. &
   DES_BC_Z_b(BCV) /= DES_BC_Z_t(BCV) &
   .OR. &
   DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
   DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
   DES_BC_Y_s(BCV) /= ZERO .AND. &
   DES_BC_Y_s(BCV) /= YLENGTH &
   .OR. &
   DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
   DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
   DES_BC_Z_b(BCV) /= ZERO .AND. &
   DES_BC_Z_b(BCV) /= ZLENGTH) THEN

! If a slit flow inlet is specified near an edge, expand the slit to
! the width of one particle diameter :
! 1) check that the inlet slit +/- a particle radius is not near either
!   domain boundary edge (south/north or bottom/top) and if not shift
!   the south/bottom location of the inlet down by a particle radius
!   and the north/top location of the inlet up by a particle radius
! 2) if the inlet slit is near the south/bottom domain edge then move
!   the south/bottom location of the inlet to the domain boundary edge
!   and the north/top location one particle diameter distance away
! 3) if the inlet slit is near the north/top domain edge then move the
!   north/top location of the inlet to the domain boundary edge and the
!   south/bottom location one particle diameter distance away
IF(DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV)) THEN

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      IF(((DES_BC_Y_s(BCV) - MAX_DIA*HALF) .GE. ZERO) .AND. &
        ((DES_BC_Y_s(BCV) + MAX_DIA*HALF) .LE. YLENGTH)) THEN
        DES_BC_Y_s(BCV) = DES_BC_Y_s(BCV) - MAX_DIA*HALF
        DES_BC_Y_n(BCV) = DES_BC_Y_n(BCV) + MAX_DIA*HALF
      ELSEIF((DES_BC_Y_s(BCV) - MAX_DIA*HALF) .LT. ZERO) THEN
        DES_BC_Y_s(BCV) = ZERO
        DES_BC_Y_n(BCV) = MAX_DIA
      ELSEIF((DES_BC_Y_n(BCV) + MAX_DIA*HALF) .GT. YLENGTH) THEN
        DES_BC_Y_s(BCV) = YLENGTH - MAX_DIA
        DES_BC_Y_n(BCV) = YLENGTH
      ENDIF
    ENDIF
  IF(DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV)) THEN
    IF(((DES_BC_Z_b(BCV) - MAX_DIA*HALF) .GE. ZERO) .AND. &
      ((DES_BC_Z_b(BCV) + MAX_DIA*HALF) .LE. ZLENGTH)) THEN
      DES_BC_Z_b(BCV) = DES_BC_Z_b(BCV) - MAX_DIA*HALF
      DES_BC_Z_t(BCV) = DES_BC_Z_t(BCV) + MAX_DIA*HALF
    ELSEIF((DES_BC_Z_b(BCV) - MAX_DIA*HALF) .LT. ZERO) THEN
      DES_BC_Z_b(BCV) = ZERO
      DES_BC_Z_t(BCV) = MAX_DIA
    ELSEIF((DES_BC_Z_t(BCV) + MAX_DIA*HALF) .GT. ZLENGTH) THEN
      DES_BC_Z_b(BCV) = ZLENGTH - MAX_DIA
      DES_BC_Z_t(BCV) = ZLENGTH
    ENDIF
  ENDIF

! Classify the boundary condition
  IF(DES_BC_X_w(BCV) == ZERO) DES_MI_CLASS(BCV_I) = 'YZw'
  IF(DES_BC_X_w(BCV) == XLENGTH) DES_MI_CLASS(BCV_I) = 'YZe'

! Inlet dimensions
  LEN1 = (DES_BC_Y_n(BCV) - DES_BC_Y_s(BCV))
  LEN2 = (DES_BC_Z_t(BCV) - DES_BC_Z_b(BCV))

  ENDIF ! End check mass inlet on YZ face: 3D

  CALL DES_BC_VEL_ASSIGN(BCV,BCV_I,LEN1,LEN2,PHASE_CNT,PHASE_LIST)

! This subroutine determines the pattern that the particles will need to
! enter the system, if any. This routine only needs to be called if a
! run is new. If a run is a RESTART_1, all of the setup information
! provided by this subroutine is will be obtained from the *_DES.RES file.
! This is done due to this routine's strong dependence on the
! RANDOM_NUMBER() subroutine.
  IF(RUN_TYPE == 'NEW') THEN
    CALL DES_MI_LAYOUT(LEN1, LEN2, BCV, BCV_I, MAX_DIA,&
      PHASE_CNT, PHASE_LIST)
  ENDIF

  ENDIF ! end if dimn == 2/else

! Verify that an inlet is not on a face that is connected to a periodic
! boundary condition. If so, write error message and exit.
  DMC = DES_MI_CLASS(BCV_I)
  IF (DES_PERIODIC_WALLS) THEN
! No XW, XE, YZw or YZe inlet with X direction periodic walls
    IF((DMC == 'XW' .OR. DMC == 'XE' .OR. &
      DMC == 'YZw' .OR. DMC == 'YZe') .AND. DES_PERIODIC_WALLS_X) THEN
      WRITE(UNIT_LOG, 1202) BCV, 'DES_PERIODIC_WALLS_X'
      WRITE(*, 1202) BCV, 'DES_PERIODIC_WALLS_X'
      CALL MFIX_EXIT(myPE)
    ENDIF
! No YS, YN, XZs or XZn inlet with Y direction periodic walls

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      IF((DMC == 'YS' .OR. DMC == 'YN' .OR. &
        DMC == 'XZs' .OR. DMC == 'XZn') .AND. DES_PERIODIC_WALLS_Y) THEN
        WRITE(UNIT_LOG, 1202)BCV, 'DES_PERIODIC_WALLS_Y'
        WRITE(*, 1202) BCV, 'DES_PERIODIC_WALLS_Y'
        CALL MFIX_EXIT(myPE)
      ENDIF
! No XYb or XYt inlet with Z direction periodic walls
      IF((DMC == 'XYb' .OR. DMC == 'XYt') .AND. DES_PERIODIC_WALLS_Z) THEN
        WRITE (UNIT_LOG, 1202) BCV, 'DES_PERIODIC_WALLS_Z'
        WRITE (*, 1202) BCV, 'DES_PERIODIC_WALLS_Z'
        CALL MFIX_EXIT(myPE)
      ENDIF
    ENDIF

! Set flags for individual mass inlets for used in the grid based search
! Flag that a X-face inlet exits
      IF(DMC == 'XW' .OR. DMC == 'XE' .OR. &
        DMC == 'YZw' .OR. DMC == 'YZe') THEN
        DES_MI_X = .TRUE.
      ENDIF
! Flag that a Y-face inlet exits
      IF(DMC == 'YS' .OR. DMC == 'YN' .OR. &
        DMC == 'XZs' .OR. DMC == 'XZn') THEN
        DES_MI_Y = .TRUE.
      ENDIF
! Flag that a Z-face inlet exits
      IF(DMC == 'XYb' .OR. DMC == 'XYt') THEN
        DES_MI_Z = .TRUE.
      ENDIF

1202 FORMAT(/1X,70('*')//, ' From: DES_MI_CLASSIFY -',/,&
  ' Message : DEM inlet can not be placed on a periodic',&
  ' boundary.',/10X,'Check DEM boundary condtion ',I3,&
  ' and ',A,'.',/1X,70('*')/)

RETURN
END SUBROUTINE DES_MI_CLASSIFY

```

```

! ~~~~~
! Module name: DES_BC_VEL_ASSIGN
!
! Purpose:
!
! Author: J.Musser
! Date: 21-Jan-10
!
! Comments:
! ~~~~~

      SUBROUTINE DES_BC_VEL_ASSIGN(BCV,BCV_I,LEN1,LEN2,PHASE_CNT,&
        PHASE_LIST)

      USE compar
      USE des_bc
      USE discretelement
      USE funits
      USE geometry
      USE param
      USE physprop

      IMPLICIT NONE

!-----
! Local variables
!-----
! passed arguments giving index information of the boundary
      INTEGER BCV_I, BCV
! Number of solid phases at bc
      INTEGER PHASE_CNT
! List of phases used in current bc
      INTEGER PHASE_LIST(MMAX)
! the length of each side of the inlet boundary
      DOUBLE PRECISION LEN1, LEN2, BCV_AREA
! the number of trial velocities to test for UI_VEL in a given iteration
      INTEGER, PARAMETER :: NUM_VEL = 100
! Dummy index
      INTEGER I
! Index of solid phases at bc
      INTEGER M, MM
! Solids volume fraction of solids phase M
      DOUBLE PRECISION EP_sM
! Temp inlet velocity for solids phase M
      DOUBLE PRECISION TMP_VEL(DIM_M)
! Minimum/maximum solids velocity at inlet. Also used in the iterative
! steps as the starting and ending velocities
      DOUBLE PRECISION MIN_VEL, MAX_VEL
! Temp variable for DES_MI_CLASS(BCV_I)
      CHARACTER*3 DMCL
! Uniform inlet velocity
      DOUBLE PRECISION UI_VEL
! Error in solids phase bulk density for phase M corresponding
! to UI_VEL compared to the user set bulk density for phase M
      DOUBLE PRECISION ERR_ROPSM
! Bulk density of phase M calculated using STP_VEL or UI_VEL
      DOUBLE PRECISION CAL_ROPSM

!--- Iterative process variables
! Counts the number of iterations performed and exits if >100

```

```

        INTEGER LC_EXIT
! Velocity minimizing the error for the PREvious and CURrent iterations
        DOUBLE PRECISION CUR_VEL, PRV_VEL
! Incremental velocity step size (delta velocity)
        DOUBLE PRECISION DELTA_VEL
! Incremental step velocity
        DOUBLE PRECISION STP_VEL
! Total error for all solid phase generated by STP_VEL
        DOUBLE PRECISION ERR_TOT
! Minimum error generated on current iteration
        DOUBLE PRECISION ERR_MIN
! Convergence tolerance
        DOUBLE PRECISION, PARAMETER :: TOL = 1.0e-4
!-----
! Initialize
        MIN_VEL = LARGE_NUMBER
        MAX_VEL = ZERO

! BC inlet area
! To calculate velocity based on specified mass/volumetric inflow and
! bulk density the inlet needs to have dimension of length^2 (area).
! In the 2D case the depth of the inlet is taken to be the maximum
! particle diameter which is consistent with how the criteria for
! maximum and minimum velocity for the boundary are defined and how
! particles are seeded for a 2D inlet (particles are seeded along a
! line that has a depth equal to the maximum particle diameter).
! Alternatively, the depth of the inlet could be taken as zlength,
! but zlength is not guaranteed to be equal to the maximum particle
! diameter.
        BCV_AREA = LEN1*LEN2

! Calculate the individual velocities for each solid phase
        DO MM = 1, PHASE_CNT
            M = PHASE_LIST(MM)
! Solids volume fraction for phase M
            EP_sM = DES_BC_ROP_s(BCV,M)/RO_s(M)
! Inlet velocity for solids phase M
            TMP_VEL(M) = ( DES_BC_VOLFLOW_s(BCV,M) / &
                BCV_AREA ) / EP_sM
! Check for min/max inlet velocity
            MIN_VEL = MIN(ABS(TMP_VEL(M)), MIN_VEL)
            MAX_VEL = MAX(ABS(TMP_VEL(M)), MAX_VEL)
        ENDDO

! Determine necessary uniform inlet velocity
        IF(MIN_VEL == MAX_VEL) THEN
            UI_VEL = MIN_VEL
        ELSE

! Initialize Values
            LC_EXIT = 0
            PRV_VEL = UNDEFINED
            CUR_VEL = ZERO

            DO WHILE (ABS(CUR_VEL - PRV_VEL)>TOL)
! Initialize Values
! Store current velocity value in previous velocity
                PRV_VEL = CUR_VEL
! Set minimum error value to a large number
                ERR_MIN = LARGE_NUMBER
! Determine step size between tested velocity values
                DELTA_VEL = (MAX_VEL-MIN_VEL)/DBLE(NUM_VEL)

```

```

! Check i=NUM_VEL velocities between MAX_VEL and MIN_VEL for one that
! minimizes the total error between calculated bulk density values
! and the values provided in the mfix.dat file. The first loop (i=1)
! acts to initialize the values of cur_vel and err_min.
      DO I = 1, (NUM_VEL+1)
! Initialize values
          STP_VEL = MIN_VEL + DELTA_VEL*(I-1)
          ERR_TOT = ZERO
! Calculate total error over all solid phases with respect to STP_VEL
          DO MM = 1, PHASE_CNT
              M = PHASE_LIST(MM)
! Calculate bulk density value based upon velocity
              CAL_ROPSM = (RO_s(M) * DES_BC_VOLFLOW_s(BCV,M)) / &
                  (STP_VEL * BCV_AREA)
              ERR_TOT = ERR_TOT+ABS(DES_BC_ROP_s(BCV,M)-CAL_ROPSM)
          ENDDO
! Compare to determine if ERR_TOT is minimum error over all STP_VEL
          IF(ERR_TOT == MIN(ERR_TOT, ERR_MIN)) THEN
              ERR_MIN = ERR_TOT
              CUR_VEL = STP_VEL
          ENDIF
! Narrow search range for next iterative set. These values only change
! if cur_vel is updated which only occurs when the current stp_vel gives
! a smaller total error than previously
              MIN_VEL = CUR_VEL - DELTA_VEL
              MAX_VEL = CUR_VEL + DELTA_VEL
          ENDDO

! Loop control to prevent hang up. * This should not be necessary *
          LC_EXIT = LC_EXIT +1
          IF(LC_EXIT > 100) THEN
              WRITE(*,1256) BCV
              EXIT
          ENDIF
      ENDDO
      UI_VEL = CUR_VEL
  ENDF

! Assign the uniform inlet velocity to each solid phase
  DMCL = DES_MI_CLASS(BCV_I)
  DO MM = 1, PHASE_CNT
      M = PHASE_LIST(MM)
      IF(DMCL == 'XW' .OR. DMCL == 'YZw') THEN
          DES_BC_U_s(BCV) = UI_VEL
      ELSEIF(DMCL == 'XE' .OR. DMCL == 'YZe') THEN
          DES_BC_U_s(BCV) = -UI_VEL
      ELSEIF(DMCL == 'YS' .OR. DMCL == 'XZs') THEN
          DES_BC_V_s(BCV) = UI_VEL
      ELSEIF(DMCL == 'YN' .OR. DMCL == 'XZn') THEN
          DES_BC_V_s(BCV) = -UI_VEL
      ELSEIF(DMCL == 'XYb') THEN
          DES_BC_W_s(BCV) = UI_VEL
      ELSEIF(DMCL == 'XYt') THEN
          DES_BC_W_s(BCV) = -UI_VEL
      ELSE
          WRITE(*,1257) BCV, DMCL
          CALL MFIX_EXIT(myPE)
      ENDIF
  ENDDO

! Output the new data values (screen/log file)
  WRITE(*,1249)
! Table Header

```

```

WRITE(*,1250) BCV
WRITE(*,1251) UI_VEL
WRITE(*,1252)
WRITE(UNIT_LOG,1250)BCV
WRITE(UNIT_LOG,1251)UI_VEL
WRITE(UNIT_LOG,1252)

! Column Labels
WRITE(*,1253)
WRITE(*,1254)
WRITE(*,1253)
WRITE(UNIT_LOG,1253)
WRITE(UNIT_LOG,1254)
WRITE(UNIT_LOG,1253)

! Fill Table Rows
DO MM = 1, PHASE_CNT
  M = PHASE_LIST(MM)
! Calculate bulk density value based upon velocity
  CAL_ROPSM = (RO_s(M) * DES_BC_VOLFLOW_s(BCV,M)) / &
    (UI_VEL * BCV_AREA)
  ERR_ROPSM = ABS(DES_BC_ROP_s(BCV,M) - CAL_ROPSM)
  WRITE(*,1255) M, DES_BC_ROP_s(BCV,M), CAL_ROPSM, ERR_ROPSM
  WRITE(*,1253)
  WRITE(UNIT_LOG,1255) M, DES_BC_ROP_s(BCV,M), CAL_ROPSM, &
    ERR_ROPSM
  WRITE(UNIT_LOG,1253)
ENDDO
WRITE(*,"(//)")
WRITE(UNIT_LOG,"(//)")

1249 FORMAT(//,5X,'From: DES_BC_VEL_ASSIGN - ')
1250 FORMAT(5X,'|<--- Boundary Condition ',I2,1X,26('-'),'>|')
1251 FORMAT(5X,'| Uniform Inlet Velocity: ',ES11.4,18(' '),'|')
1252 FORMAT(5X,'| Adjusted DES_BC_ROP_s Values',25(' '),'|')
1253 FORMAT(5X,'|',54('-'),'|')
1254 FORMAT(5X,'|',3X,'Phase',3X,'|',2X,'Specified',2X,'|',2X,&
  'Calculated',2X,'|',2X,'ABS Error',2X,'|')
1255 FORMAT(5X,'|',4X,I2,5X,'|',1X,ES11.4,1X,'|',1X,ES11.4,2X,'|',&
  1X,ES11.4,1X,'|')

1256 FORMAT(/1X,70('*')//,' From: DES_BC_VEL_ASSIGN -',/,&
  ' Message : Tolerance not met on uniform inlet velocity for',&
  /10X,'boundary ', I3, /1X,70('*')/)

1257 FORMAT(/1X,70('*')//,' From: DES_BC_VEL_ASSIGN -',/,&
  ' Message : INVALID BOUNDARY CLASSIFICATION FOR BOUNDARY',I3,&
  /10X, 'with classification ',A,/1X,70('*')/)

RETURN
END SUBROUTINE DES_BC_VEL_ASSIGN

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[illegible]

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        INTEGER TMP_INT
! Temp variable for DES_MI_CLASS(BCV_I)
        CHARACTER*3 DMCL

! lower threshold velocities that will work given the flow boundary
! specifications:
! lower maximum inlet particle velocity (MAXIPV); above which particles
! enter fast enough not to require additional handling
! lowest minimum inlet particle velocity (MINIPV) below which particles
! do not enter fast enough to meet the massflow rate and an error is
! flagged; above minipv and below maxipv the particle inlet conditions
! are adequate but must be carefully controlled
        DOUBLE PRECISION MAXIPV, MINIPV

!-----

        IF(LEN2 == ZERO)THEN      ! 2D domain
!-----
                TMP_LEN1 = FLOOR(real(LEN1/MAX_DIA))
                TMP_LEN2 = ZERO
! notes :
!   dtsolid*pi_factor(:)      = time elapsed between particle injections
!                               = des_mi_time(:)
!   d_p0/(dtsolid*pi_factor(:)) = approx velocity needed to move one particle
!                               diameter at the specified mass flow rate
!   ceiling(tmp_len1/2)       = the minimum no. of particles that can
!                               be arranged along the inlet so that an
!                               additional particle cannot fit
!   k > 1 represents cases with more than 1 particles injected in a single
!   solids timestep

                K = PI_COUNT(BCV_I)
                MAXIPV = MAX_DIA/( DTSOLID*dble(PI_FACTOR(BCV_I))*&
                        dble( FLOOR( CEILING( real(TMP_LEN1)/2.0 ) /real(K) ) ))
                MINIPV = MAX_DIA/( DTSOLID*dble(PI_FACTOR(BCV_I))*&
                        dble( FLOOR( real(TMP_LEN1)/real(K) ) ))
                IF (MINIPV .LT. SMALL_NUMBER) MINIPV = ZERO

                DMCL = DES_MI_CLASS(BCV_I)

! Check each solid phase to determine how the particles are to be
! placed and if the mass inflow conditions can be achieved.
                IF(DMCL == 'XW' .OR. DMCL == "XE")THEN
                        BC_VEL = ABS(DES_BC_U_s(BCV))
                ELSEIF(DMCL == 'YS' .OR. DMCL == "YN")THEN
                        BC_VEL = ABS(DES_BC_V_s(BCV))
                ENDIF

! The bc velocity is lowered by a small number to prevent possible
! issues with the mantissa truncation
                IF(MAXIPV .LE. (BC_VEL - SMALL_NUMBER))THEN
! The inlet velocity is sufficient to permit random placement of the new
! particles without risk of overlap
                        PARTICLE_PLCMNT(BCV_I) = 'RAND'
! Override the random placement for an ordered inlet
                        IF(FORCE_ORD_BC) PARTICLE_PLCMNT(BCV_I) = 'ORDR'
                        ELSEIF(MINIPV .LE. (BC_VEL - SMALL_NUMBER) .AND. &
                                (BC_VEL .LT. MAXIPV + SMALL_NUMBER)) THEN
! Then inlet velocity will require that the new particles be placed with
! order to prevent overlap.
                                PARTICLE_PLCMNT(BCV_I) = 'ORDR'
                        ELSE
! The inlet velocity is too low to satisfy the other inlet conditions.

```

```

! Determine maximum possible ROP_s values that will satisfy the inlet
! conditions. Flag error, prompt with new values, and exit.
      WRITE(UNIT_LOG,1300) BCV
      WRITE(*,1300) BCV
      DO MM = 1, PHASE_CNT
        M = PHASE_LIST(MM)
! Even though the system is 2D, an area of the inlet is needed for
! the following calculation. This 'depth' is taken as max_dia.
        MAX_ROPs = (DES_BC_VOLFLOW_s(BCV,M)*RO_s(M)) / &
          (MINIPV * LEN1 * MAX_DIA)
        WRITE(UNIT_LOG,1301) BCV, M, MAX_ROPs
        WRITE(*,1301) BCV, M, MAX_ROPs
      ENDDO
      WRITE(UNIT_LOG,1302)
      WRITE(*,1302)
      CALL MFIX_EXIT(myPE)
    ENDIF

    IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR') THEN
! In 2D calculate the approx. particle line density (e.g., the no. of
! particles along the inlet) needed to achieve the specified particle
! mass flow rate and particle velocity;
      TMP_FACTOR = CEILING(real(MAX_DIA / &
        (dble(PI_FACTOR(BCV_I)) * DTSOLID * ABS(BC_VEL))))
      ALLOCATE( MI_ORDER(BCV_I)%VALUE( TMP_FACTOR ) )
      ALLOCATE( I_OF_MI(BCV_I)%VALUE( TMP_FACTOR ) )

! Initialize
      MI_ORDER(BCV_I)%VALUE(:) = -1
      MI_FACTOR(BCV_I) = 1
! Dimension of grid cell; this may be larger than than the particle
! diameter but not smaller
      MI_WINDOW(BCV_I) = LEN1/dble(TMP_FACTOR)
      DO I = 1, TMP_FACTOR
        I_OF_MI(BCV_I)%VALUE(I) = I - 1
      ENDDO

! Construct an array of integers from 1 to TMP_FACTOR in a random
! order. This is used when placing new particles.
      LL = 1
      DO WHILE (MI_ORDER(BCV_I)%VALUE(TMP_FACTOR) .EQ. -1)
        CALL RANDOM_NUMBER(TMP_DP)
        TMP_INT = CEILING(real(TMP_DP*dble(TMP_FACTOR)))
        DO LC = 1, LL
          IF(TMP_INT .EQ. MI_ORDER(BCV_I)%VALUE(LC) ) EXIT
          IF(LC .EQ. LL) THEN
            MI_ORDER(BCV_I)%VALUE(LC) = TMP_INT
            LL = LL + 1
          ENDIF
        ENDDO
      ENDDO
      ENDIF
! endif particle_plcmnt(bcv_i) == 'ordr'

    ELSEIF(LEN2 /= ZERO) THEN ! 3D domain
!-----
      TMP_LEN1 = FLOOR(real(LEN1/MAX_DIA))
      TMP_LEN2 = FLOOR(real(LEN2/MAX_DIA))

      K = PI_COUNT(BCV_I)
! In the 3D case the calculation for MAXIPV is conservative. That is,
! the actual bc velocity could be somewhat lower than the calculated
! value of MAXIPV and still allow for random particle placement

```



```

MAXIPV = MAX_DIA/( DTSOLID*dble(PI_FACTOR(BCV_I)) * &
  dble( FLOOR( CEILING( &
    real(TMP_LEN1*TMP_LEN2)/2.0 ) /real(K) ) ))
! The cutoff is associated with square packing of disks on a plane
! A lower velocity would be possible with hexagonal packing
MINIPV = MAX_DIA/( DTSOLID*dble(PI_FACTOR(BCV_I)) * &
  dble( FLOOR( real(TMP_LEN1*TMP_LEN2)/real(K) ) ))

IF (MINIPV .LT. SMALL_NUMBER) MINIPV = ZERO

DMCL = DES_MI_CLASS(BCV_I)
! Check each solid phase to determine how the particles are to be
! placed or if the mass inflow conditions can be achieved.
IF(DMCL == 'YZe' .OR. DMCL == "YZw") THEN
  BC_VEL = ABS(DES_BC_U_s(BCV))
ELSEIF(DMCL == 'XZs' .OR. DMCL == "XZn") THEN
  BC_VEL = ABS(DES_BC_V_s(BCV))
ELSEIF(DMCL == 'XYb' .OR. DMCL == "XYt") THEN
  BC_VEL = ABS(DES_BC_W_s(BCV))
ENDIF
! The bc velocity is lowered by a small number to prevent possible
! issues with the mantissa truncation
IF(MAXIPV .LE. (ABS(BC_VEL) - SMALL_NUMBER)) THEN
! The inlet velocity is sufficient to permit random placement of the new
! particles without risk of overlap
  PARTICLE_PLCMNT(BCV_I) = 'RAND'
! Override the random placement for an ordered inlet
  IF(FORCE_ORD_BC) PARTICLE_PLCMNT(BCV_I) = 'ORDR'
ELSEIF(MINIPV .LE. (BC_VEL - SMALL_NUMBER) .AND. &
  (BC_VEL .LT. MAXIPV + SMALL_NUMBER)) THEN
! Then inlet velocity will require that the new particles be placed with
! order to prevent overlap.
  PARTICLE_PLCMNT(BCV_I) = 'ORDR'
ELSE
! The inlet velocity is too low to satisfy the other inlet conditions.
! Determine maximum possible ROP_s values that will satisfy the inlet
! conditions. Flag error, propt with new values, and exit.
  WRITE(UNIT_LOG,1300)BCV; WRITE(*,1300)BCV
  DO MM = 1, PHASE_CNT
    M = PHASE_LIST(MM)
    MAX_ROPs = (DES_BC_VOLFLOW_s(BCV,M)*RO_s(M)) / &
      (MINIPV * LEN1 * LEN2)
    WRITE(UNIT_LOG,1301)BCV,M,MAX_ROPs
    WRITE(*,1301)BCV,M,MAX_ROPs
  ENDDO
  WRITE(UNIT_LOG,1302)
  WRITE(*,1302)
  CALL MFIX_EXIT(myPE)
ENDIF

IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR') THEN
! In 3D calculate the the number of grid cells within the inlet face
! with length dimension of 1 particle diameter
  TMP_FACTOR = TMP_LEN1 * TMP_LEN2
  ALLOCATE( MI_ORDER(BCV_I)%VALUE( TMP_FACTOR ) )
  ALLOCATE( I_OF_MI(BCV_I)%VALUE( TMP_FACTOR ) )
  ALLOCATE( J_OF_MI(BCV_I)%VALUE( TMP_FACTOR ) )

! Initialize
  MI_ORDER(BCV_I)%VALUE(:) = -1
  MI_FACTOR(BCV_I) = 1
! Dimension of grid cell; this may be larger than than the particle
! diameter but not smaller:

```

```

! if len1/tmp_len1 < len2/tmp_len2, len1/tmp_len1*tmp_len2 < len2 or
! if len1/tmp_len1 > len2/tmp_len2, len2/tmp_len2*tmp_len1 < len1
  MI_WINDOW(BCV_I) = MIN(LEN1/TMP_LEN1, LEN2/TMP_LEN2)

  DO I = 1, TMP_LEN1
    DO J = 1, TMP_LEN2
      IJ = J + (I-1)*TMP_LEN2
      I_OF_MI(BCV_I)%VALUE(IJ) = I - 1
      J_OF_MI(BCV_I)%VALUE(IJ) = J - 1
    ENDDO
  ENDDO

! Construct an array of integers from 1 to TMP_FACTOR in a random
! order. This is used when placing new particles.
  LL = 1
  DO WHILE (MI_ORDER(BCV_I)%VALUE(TMP_FACTOR) .EQ. -1)
    CALL RANDOM_NUMBER(TMP_DP)
    TMP_INT = CEILING(real(TMP_DP*dble(TMP_FACTOR)))
    DO LC = 1, LL
      IF(TMP_INT .EQ. MI_ORDER(BCV_I)%VALUE(LC) )EXIT
      IF(LC .EQ. LL)THEN
        MI_ORDER(BCV_I)%VALUE(LC) = TMP_INT
        LL = LL + 1
      ENDIF
    ENDDO
  ENDDO
  ENDF ! endif particle_plcmnt(bcv_i) == 'ordr'

ENDIF ! endif len2 == zero

WRITE(*,1303) BCV, LEN1, LEN2, TMP_LEN1, TMP_LEN2,&
  MAXIPV, MINIPV, PARTICLE_PLCMNT(BCV_I)

1300 FORMAT(/1X,70('*')//,' From: DES_MI_LAYOUT -',/,&
  ' Message: DES_BC_ROP_s values for BC ',I3,' are set too ',&
  'high.',/,10X,'The MAXIMUM values for the supplied inlet ',&
  'conditions are:')

1301 FORMAT(10X,'DES_BC_ROP_s(',I3,',',I3,') < ',F9.4)

1302 FORMAT(1X,70('*'))

1303 FORMAT(5X,'From: DES_MI_LAYOUT - BC: ', I3, /7X,&
  'LEN1 = ', ES17.5,4X, ' LEN2 = ', ES17.5,/7X,&
  'TMP_LEN1 = ', I6,11X, ' TMP_LEN2 = ', I6,/7X,&
  'MAXIPV = ', ES17.5,2X, ' MINIPV = ', ES17.5,/7X,&
  'PLCMNT = ',3X,A,/)

RETURN
END SUBROUTINE DES_MI_LAYOUT

```

```

! ~~~~~
! Module name: DES_MI_CELLS
!
! Purpose:
!   Locate the i, j, k position of the cells encompassing the DES
!   mass inlet BC so that when particles are injected into the system,
!   a complete grid search is not necessary to prevent/determine:
!     1) the injected particle from overlapping with an existing
!        particle nearby when particle_plcmnt = 'rand'
!     2) the i, j, k indices of the newly injected particle on the
!        eulerian grid defined by imax, jmax, kmax
!
! Author: J.Musser
!
! Date: 5-Oct-09
!
! Comments:
! ~~~~~
!
! SUBROUTINE DES_MI_CELLS(BCV, BCV_I)
!
!   USE des_bc
!   USE discretelement
!   USE geometry
!
!   IMPLICIT NONE
!
! -----
! Local variables
! -----
! passed arguments giving index information of the boundary
!   INTEGER BCV_I, BCV
!
!   INTEGER I,J,K
! dummy variable for length calculations
!   DOUBLE PRECISION LOCATION
! -----
!
! IF(DES_BC_X_w(BCV) == DES_BC_X_e(BCV)) THEN
!   IF(DES_BC_X_w(BCV) == ZERO) GS_ARRAY(BCV_I,1:2) = 1
!   IF(DES_BC_X_w(BCV) == XLLENGTH) GS_ARRAY(BCV_I,1:2) = IMAX2
! ELSE
! note dx(1) = length of ghost cell (x < zero)
!   I=2; LOCATION = ZERO
!   DO WHILE (LOCATION <= XLLENGTH)
!     IF((DES_BC_X_w(BCV) >= LOCATION) .AND. &
!       (DES_BC_X_w(BCV) < LOCATION + DX(I))) THEN
!       GS_ARRAY(BCV_I,1) = I
!     ENDIF
!     IF((DES_BC_X_e(BCV) >= LOCATION) .AND. &
!       (DES_BC_X_e(BCV) < LOCATION + DX(I))) THEN
!       GS_ARRAY(BCV_I,2) = I
!     EXIT
!   ENDIF
!   LOCATION = LOCATION + DX(I)
!   I=I+1
! ENDDO
! ENDIF
!
! IF(DES BC Y s(BCV) == DES BC Y n(BCV)) THEN

```

```

        IF (DES_BC_Y_s (BCV) == ZERO) GS_ARRAY (BCV_I, 3:4) = 1
        IF (DES_BC_Y_s (BCV) == YLENGTH) GS_ARRAY (BCV_I, 3:4) = JMAX2
    ELSE
! note dy(1) = length of ghost cell (y < zero)
        J=2; LOCATION = ZERO
        DO WHILE (LOCATION <= YLENGTH)
            IF ((DES_BC_Y_s (BCV) >= LOCATION) .AND. &
                (DES_BC_Y_s (BCV) < LOCATION + DY(J))) THEN
                GS_ARRAY (BCV_I, 3) = J
            ENDIF
            IF ((DES_BC_Y_n (BCV) >= LOCATION) .AND. &
                (DES_BC_Y_n (BCV) < LOCATION + DY(J))) THEN
                GS_ARRAY (BCV_I, 4) = J
            EXIT
            ENDIF
            LOCATION = LOCATION + DY(J)
            J=J+1
        ENDDO
    ENDIF

    IF (DIMN == 2) THEN
        GS_ARRAY (BCV_I, 5:6) = 1
    ELSE
        IF (DES_BC_Z_b (BCV) == DES_BC_Z_t (BCV)) THEN
            IF (DES_BC_Z_b (BCV) == ZERO) GS_ARRAY (BCV_I, 5:6) = 1
            IF (DES_BC_Z_b (BCV) == ZLENGTH) GS_ARRAY (BCV_I, 5:6) = KMAX2
        ELSE
            K=2; LOCATION = ZERO
            DO WHILE (LOCATION <= ZLENGTH)
                IF ((DES_BC_Z_b (BCV) >= LOCATION) .AND. &
                    (DES_BC_Z_b (BCV) < LOCATION + DZ(K))) THEN
                    GS_ARRAY (BCV_I, 5) = K
                ENDIF
                IF ((DES_BC_Z_t (BCV) >= LOCATION) .AND. &
                    (DES_BC_Z_t (BCV) < LOCATION + DZ(K))) THEN
                    GS_ARRAY (BCV_I, 6) = K
                EXIT
                ENDIF
                LOCATION = LOCATION + DZ(K)
                K=K+1
            ENDDO
        ENDIF
    ENDIF

    RETURN
END SUBROUTINE DES_MI_CELLS

```

```
! ~~~~~!  
! Module name: DES_MO_CLASSIFY  
!  
! Purpose:  
!  
! Author: J.Musser Date: 5-Oct-09  
!  
! Comments:  
!  
! ~~~~~!
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        DES_BC_Z_b(BCV) /= DES_BC_Z_t(BCV) &
    .OR. &
        DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
        DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        DES_BC_Y_s(BCV) /= ZERO .AND. &
        DES_BC_Y_s(BCV) /= YLENGTH &
    .OR. &
        DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
        DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
        DES_BC_Z_b(BCV) /= ZERO .AND. &
        DES_BC_Z_b(BCV) /= ZLENGTH) THEN

        DES_MO_X = .TRUE.
        IF (DES_BC_X_w(BCV) == ZERO) DES_MO_CLASS(BCV_I) = 'XW'
        IF (DES_BC_X_w(BCV) == XLENGTH) DES_MO_CLASS(BCV_I) = 'XE'

    ENDIF
! End check mass outlet on YZ face: 3D

! Check mass inlet on XZ face: 3D
! -----
    IF (DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
        DES_BC_Z_b(BCV) /= DES_BC_Z_t(BCV) &
    .OR. &
        DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
        DES_BC_X_w(BCV) /= ZERO .AND. &
        DES_BC_X_w(BCV) /= XLENGTH &
    .OR. &
        DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
        DES_BC_Z_b(BCV) /= ZERO .AND. &
        DES_BC_Z_b(BCV) /= ZLENGTH) THEN

        DES_MO_Y = .TRUE.
        IF (DES_BC_Y_s(BCV) == ZERO) DES_MO_CLASS(BCV_I) = 'YS'
        IF (DES_BC_Y_s(BCV) == YLENGTH) DES_MO_CLASS(BCV_I) = 'YN'

    ENDIF
! End check mass outlet on XZ face: 3D

! Check mass inlet on XY face: 3D
! -----
    IF (DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
        DES_BC_X_w(BCV) /= DES_BC_X_e(BCV) .AND. &
        DES_BC_Y_s(BCV) /= DES_BC_Y_n(BCV) &
    .OR. &
        DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
        DES_BC_X_w(BCV) == DES_BC_X_e(BCV) .AND. &
        DES_BC_X_w(BCV) /= ZERO .AND. &
        DES_BC_X_w(BCV) /= XLENGTH &
    .OR. &
        DES_BC_Z_b(BCV) == DES_BC_Z_t(BCV) .AND. &
        DES_BC_Y_s(BCV) == DES_BC_Y_n(BCV) .AND. &
        DES_BC_Y_s(BCV) /= ZERO .AND. &
        DES_BC_Y_s(BCV) /= YLENGTH) THEN

        DES_MO_Z = .TRUE.
        IF (DES_BC_Z_b(BCV) == ZERO) DES_MO_CLASS(BCV_I) = 'ZB'
        IF (DES_BC_Z_b(BCV) == ZLENGTH) DES_MO_CLASS(BCV_I) = 'ZT'

```

```

ENDIF
! End check mass outlet on XY face: 3D

ENDIF ! endif dimn == 2

! Verify that an inlet is not on a face that is connected to a periodic
! boundary condition. If so, write error message and exit.
! No Xew outlet with X direction periodic walls
IF((DES_MO_CLASS(BCV_I) == 'XW' .OR. DES_MO_CLASS(BCV_I) == 'XE') &
   .AND. DES_PERIODIC_WALLS_X) THEN
  WRITE (UNIT_LOG, 1500) BCV, 'DES_PERIODIC_WALLS_X'
  WRITE (*, 1500) BCV, 'DES_PERIODIC_WALLS_X'
  CALL MFIX_EXIT(myPE)
ENDIF
! No Ysn outlet with Y direction periodic walls
IF((DES_MO_CLASS(BCV_I) == 'YS' .OR. DES_MO_CLASS(BCV_I) == 'YN') &
   .AND. DES_PERIODIC_WALLS_Y) THEN
  WRITE (UNIT_LOG, 1500) BCV, 'DES_PERIODIC_WALLS_Y'
  WRITE (*, 1500) BCV, 'DES_PERIODIC_WALLS_Y'
  CALL MFIX_EXIT(myPE)
ENDIF
! No Zbt outlet with Z direction periodic walls
IF((DES_MO_CLASS(BCV_I) == 'ZB' .OR. DES_MO_CLASS(BCV_I) == 'ZT') &
   .AND. DES_PERIODIC_WALLS_Z) THEN
  WRITE (UNIT_LOG, 1500) BCV, 'DES_PERIODIC_WALLS_Z'
  WRITE (*, 1500) BCV, 'DES_PERIODIC_WALLS_Z'
  CALL MFIX_EXIT(myPE)
ENDIF

1500 FORMAT(/1X,70('*'))//,' From: DES_MI_CLASSIFY -',/10X,&
      'DEM outlets can not be placed on a periodic boundary.',/10X,&
      'Check DEM boundary condtion ',I2,' and ',A,'.',/1X,70('*'))

RETURN
END SUBROUTINE DES_MO_CLASSIFY

```

```

! ~~~~~
! Module name: DES_MIO_PERIODIC
!
! Purpose: ! Verify that any inlet or outlet is placed at least
! "SPACER" distance away from a periodic boundary condition. This
! will prevent any particle that crossing a periodic boundary from
! being moved into contact with an entering or exiting particle.
! This is necessary since particles are not incrementally moved
! across a periodic boundary.
!
! Author: J.Musser
!
! Date: 22-Dec-09
!
! Comments:
! ~~~~~

SUBROUTINE DES_MIO_PERIODIC(BCV,BCV_I,CLASS, MAX_DIA)

  USE compar
  USE des_bc
  USE discretelement
  USE funits
  USE geometry
  USE physprop

  IMPLICIT NONE

!-----
! Local variables
!-----

! boundary classification of inlet or outlet (MI or MO)
  CHARACTER*2 CLASS

! boundary classification of inlet or outlet (full text for messages)
  CHARACTER*6 IO_ID

! value of DES_MI/MO_CLASS (boundary plane that MI or MO is
! located on)
  CHARACTER*3 DMC

  INTEGER BCV ! absolute boundary condition number
  INTEGER BCV_I ! index boundary condtion number

! Max diameter of incoming particles at bc
  DOUBLE PRECISION MAX_DIA

! buffer space around inlets and outlets with boardering periodic
! boundary conditions
  DOUBLE PRECISION SPACER

!-----

  SPACER = 1.05d0 * MAX_DIA

  IF(CLASS == 'MI')THEN
    DMC = DES_MI_CLASS(BCV_I)
    IO_ID = "inlet"
  ELSE

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        DMC = DES_MO_CLASS(BCV_I)
        IO_ID = "outlet"
    ENDIF

    IF(DMC == 'XW' .OR. DMC == 'XE' .OR. & ! 2D inlet \ 2D-3D outlet
        DMC == 'YZw' .OR. DMC == 'YZe') THEN ! 3D inlet

        IF(DES_PERIODIC_WALLS_Y) THEN
            IF(DES_BC_Y_s(BCV) < SPACER .OR. &
                DES_BC_Y_n(BCV) > (YLENGTH - SPACER)) THEN
                WRITE(UNIT_LOG, 1600) IO_ID, BCV, 'Y'
                WRITE(*, 1600) IO_ID, BCV, 'Y'
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF

        IF(DES_PERIODIC_WALLS_Z) THEN
            IF(DES_BC_Z_b(BCV) < SPACER .OR. &
                DES_BC_Z_t(BCV) > (ZLENGTH - SPACER)) THEN
                WRITE(UNIT_LOG, 1600) IO_ID, BCV, 'Z'
                WRITE(*, 1600) IO_ID, BCV, 'Z'
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF
    ENDIF

    IF(DMC == 'YS' .OR. DMC == 'YN' .OR. & ! 2D inlet \ 2D-3D outlet
        DMC == 'XZs' .OR. DMC == 'XZn') THEN ! 3D inlet

        IF(DES_PERIODIC_WALLS_X) THEN
            IF(DES_BC_X_w(BCV) < SPACER .OR. &
                DES_BC_X_e(BCV) > (XLENGTH - SPACER)) THEN
                WRITE(UNIT_LOG, 1600) IO_ID, BCV, 'X'
                WRITE(*, 1600) IO_ID, BCV, 'X'
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF

        IF(DES_PERIODIC_WALLS_Z) THEN
            IF(DES_BC_Z_b(BCV) < SPACER .OR. &
                DES_BC_Z_t(BCV) > (ZLENGTH - SPACER)) THEN
                WRITE(UNIT_LOG, 1600) IO_ID, BCV, 'Z'
                WRITE(*, 1600) IO_ID, BCV, 'Z'
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF
    ENDIF

    IF(DMC == 'XYb' .OR. DMC == 'XYt' .OR. & ! 3D inlet
        DMC == 'ZB' .OR. DMC == 'ZT') THEN ! 3D outlet

        IF(DES_PERIODIC_WALLS_X) THEN
            IF(DES_BC_X_w(BCV) < SPACER .OR. &
                DES_BC_X_e(BCV) > (XLENGTH - SPACER)) THEN
                WRITE(UNIT_LOG, 1600) IO_ID, BCV, 'X'
                WRITE(*, 1600) IO_ID, BCV, 'X'
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF

        IF(DES_PERIODIC_WALLS_Y) THEN
            IF(DES_BC_Y_s(BCV) < SPACER .OR. &
                DES_BC_Y_n(BCV) > (YLENGTH - SPACER)) THEN
                WRITE(UNIT_LOG, 1600) IO_ID, BCV, 'Y'
                WRITE(*, 1600) IO_ID, BCV, 'Y'
                CALL MFIX_EXIT(myPE)
            ENDIF
        ENDIF
    ENDIF

```

```
ENDIF

1600 FORMAT(/1X,70('*')//, ' From: CHECK_DES_BC -',/,&
      ' Message: DES ',A,' boundary ',I3,' is too close to',&
      ' DES_PERIODIC_WALLS_',A,'.',/1X,70('*')/)

RETURN
END SUBROUTINE DES_MIO_PERIODIC
```

```
!vvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvvv!  
!  
! Module name: DES_MASS_INLET(BCV_I) !  
!  
! Purpose: This routine fills in the necessary information for new !  
! particles entering the system. !  
!  
!  
! Author: J.Musser Date: 13-Jul-09 !  
!  
! Comments: !  
!  
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
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! Check to see if MAX_PIS has been exceeded, if so, STOP
IF(PIS .GE. MAX_PIS) THEN
  WRITE(UNIT_LOG, 1000)
  WRITE(*,1000)
  CALL MFIX_EXIT(myPE)
ENDIF

! Find the first free space in the particle existence array
DO NP = LS, MAX_PIS
  IF(.NOT.PEA(NP,1)) THEN
    LS = NP
    EXIT
  ENDIF
ENDDO

! Set the flag in the particle existence array
PEA(NP,1) = .TRUE.

! Set the flag that the particle is new. This allows it to be ignored
! by various subroutines
PEA(NP,2) = .TRUE.

! Increment the particle in system value by one
PIS = PIS + 1

! Obtain a mass phase to assign to the incoming particle
IF(DES_BC_POLY(BCV_I)) THEN
  CALL RANDOM_NUMBER(RAND)
! Scale and convert random number to an interger
  RAND_I = CEILING(dble(NUMFRAC_LIMIT)*RAND)
  M = DES_BC_POLY_LAYOUT(BCV_I,RAND_I)
ELSE
  M = DES_BC_POLY_LAYOUT(BCV_I,1)
ENDIF

! Set the initial velocity values
DES_VEL_OLD(NP,1) = DES_BC_U_s(BCV)
DES_VEL_OLD(NP,2) = DES_BC_V_s(BCV)
IF(DIMN == 3) DES_VEL_OLD(NP,3) = DES_BC_W_s(BCV)

DES_VEL_NEW(NP,:) = DES_VEL_OLD(NP,:)

! Set the initial angular velocity values
OMEGA_OLD(NP,:) = 0
OMEGA_NEW(NP,:) = 0

! Set the particle radius value
DES_RADIUS(NP) = (D_P0(M) * HALF)

! Set the particle density value
RO_Sol(NP) = RO_S(M)

! Set the particle mass phase
PIJK(NP,5) = M

! Calculate the new particle's Volume, Mass, OMOI
PVOL(NP) = (4.0d0/3.0d0) * PI * DES_RADIUS(NP)**3
PMASS(NP) = PVOL(NP) * RO_Sol(NP)
OMOI(NP) = 5.d0 / (2.d0 * PMASS(NP) * DES_RADIUS(NP)**2)

! Set the initial position values based on mass inlet class
CALL DES_PLACE_NEW_PARTICLE(NP, BCV_I)

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DES_POS_NEW(NP,:) = DES_POS_OLD(NP,:)

XPOS = DES_POS_NEW(NP,1)
YPOS = DES_POS_NEW(NP,2)
IF (DIMN == 3) THEN
    ZPOS = DES_POS_NEW(NP,3)
ENDIF

! Determine the i, j, k indices of the cell containing the new
! particle(s) by checking the cells near the mass inlet using
! GS_ARRAY. Note the indices will place the particle in a ghost
! cell.
! -----
DO I = GS_ARRAY(BCV_I,1), GS_ARRAY(BCV_I,2)
    IF(XPOS < XE(1)) THEN
        PIJK(NP,1) = 1
        EXIT
    ELSEIF(XPOS >= XE(IMAX1)) THEN
        PIJK(NP,1) = IMAX2
        EXIT
    ELSEIF((XPOS >= XE(I-1)) .AND. (XPOS < XE(I))) THEN
        PIJK(NP,1) = I
        EXIT
    ENDIF
ENDDO

DO J = GS_ARRAY(BCV_I,3), GS_ARRAY(BCV_I,4)
    IF(YPOS < YN(1)) THEN
        PIJK(NP,2) = 1
        EXIT
    ELSEIF(YPOS >= YN(JMAX1)) THEN
        PIJK(NP,2) = JMAX2
        EXIT
    ELSEIF((YPOS >= YN(J-1)) .AND. (YPOS < YN(J))) THEN
        PIJK(NP,2) = J
        EXIT
    ENDIF
ENDDO

IF(DIMN == 2) THEN
    PIJK(NP,3) = 1
ELSE
    DO K = GS_ARRAY(BCV_I,5), GS_ARRAY(BCV_I,6)
        IF(ZPOS < ZT(1)) THEN
            PIJK(NP,3) = 1
            EXIT
        ELSEIF(ZPOS >= ZT(KMAX1)) THEN
            PIJK(NP,3) = KMAX2
            EXIT
        ELSEIF((ZPOS >= ZT(K-1)) .AND. (ZPOS < ZT(K))) THEN
            PIJK(NP,3) = K
            EXIT
        ENDIF
    ENDDO
ENDIF

! Update the PIC array for new particles so that any subsequent
! particles that are to be injected will be checked to prevent
! overlap with previously injected particles
I = PIJK(NP,1)
J = PIJK(NP,2)
K = PIJK(NP,3)
IJK = FUNIJK(I,J,K)

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```

      PIJK(NP,4) = IJK

      IF (ASSOCIATED(PIC(I,J,K)%P)) THEN
        NPG = SIZE(PIC(I,J,K)%P)
        ALLOCATE( HOLDER (NPG) )

! store the particle no. id of all particles at the ijk location
        TMPI = 1
        DO LL = 1, NPG
          HOLDER(TMPI) = PIC(I,J,K)%P(LL)
          TMPI = TMPI + 1
        ENDDO
        DEALLOCATE(PIC(I,J,K)%P)

! essentially increasing the no. of particles at the ijk location by 1
        ALLOCATE(PIC(I,J,K)%P(TMPI))
        DO LL = 1, TMPI - 1
          PIC(I,J,K)%P(LL) = HOLDER(LL)
        ENDDO
! storing the new particle no. id in the list
        PIC(I,J,K)%P(TMPI) = NP
        DEALLOCATE(HOLDER)
      ELSE
! no other particles were at this ijk location
        TMPI = 1
        ALLOCATE(PIC(I,J,K)%P(TMPI))
        PIC(I,J,K)%P(TMPI) = NP
      ENDIF
      PINC(IJK) = TMPI

! If using des_neighbor_search option 4 (cell/grid based search) then
! determine the i,j,k indices of the cell containing the new particle
! based on the mesh for the grid based search. If cell is outside the
! domain then either set the index to 1 or add 2 to the index to
! account for ghost cells.
! Note that this section is probably unnecessary since the routine
! particles_in_cell will pickup the same information before neighbor
! search is ever called and it is only in the neighbor search routine
! that this information should be needed
! -----
      IF (DES_NEIGHBOR_SEARCH .EQ. 4) THEN
! determine size of the mesh
        SIZEDX = XLENGTH/DESGRIDSEARCH_IMAX
        SIZEDY = YLENGTH/DESGRIDSEARCH_JMAX
        IF (DIMN .EQ. 2) THEN
          SIZEDZ = ONE
        ELSE
          SIZEDZ = ZLENGTH/DESGRIDSEARCH_KMAX
        ENDIF

        IF (XPOS < 0) THEN
          I = 1
        ELSEIF (XPOS >= XLENGTH) THEN
          I = DESGS_IMAX2
        ELSE
          I = INT(XPOS/SIZEDX)+2
        ENDIF

        IF (YPOS < 0 ) THEN
          J = 1
        ELSEIF (YPOS >= YLENGTH) THEN
          J = DESGS_JMAX2

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ELSE
    J = INT(YPOS/SIZEDY)+2
ENDIF

IF (DIMN .EQ. 2) THEN
    K = 1
ELSE
    IF (ZPOS < 0 ) THEN
        K = 1
    ELSEIF (ZPOS >= ZLENGTH) THEN
        K = DESGS_KMAX2
    ELSE
        K = INT(ZPOS/SIZEDZ)+2
    ENDIF
ENDIF

DESGRIDSEARCH_PIIK(NP,1) = I
DESGRIDSEARCH_PIIK(NP,2) = J
DESGRIDSEARCH_PIIK(NP,3) = K

! Update the DESGRIDSEARCH_PIC array for new particles. Note that
! is not needed to prevent subsequent particles that are injected
! from overlapping with previous particles as the variable PIC is
! used for that.
IF (ASSOCIATED(DESGRIDSEARCH_PIC(I,J,K)%P)) THEN
    NPG = SIZE(DESGRIDSEARCH_PIC(I,J,K)%P)
    ALLOCATE( HOLDER (NPG) )

! store the particle no. id of all particles at the ijk location
    TMPI = 1
    DO LL = 1, NPG
        HOLDER(TMPI) = DESGRIDSEARCH_PIC(I,J,K)%P(LL)
        TMPI = TMPI + 1
    ENDDO
    DEALLOCATE(DESGRIDSEARCH_PIC(I,J,K)%P)

! essentially increasing the no. of particles at the ijk location by 1
    ALLOCATE(DESGRIDSEARCH_PIC(I,J,K)%P(TMPI))
    DO LL = 1, TMPI - 1
        DESGRIDSEARCH_PIC(I,J,K)%P(LL) = HOLDER(LL)
    ENDDO

! storing the new particle no. id in the list
    DESGRIDSEARCH_PIC(I,J,K)%P(TMPI) = NP
    DEALLOCATE(HOLDER)
ELSE
! no other particles were at this ijk location
    TMPI = 1
    ALLOCATE(DESGRIDSEARCH_PIC(I,J,K)%P(TMPI))
    DESGRIDSEARCH_PIC(I,J,K)%P(TMPI) = NP
ENDIF
ENDIF ! end if des_neighbor_search = 4

ENDDO ! end loop over the no. of injected particles (NP)

1000 FORMAT(/1X,70('*')//,' From: DES_MASS_INLET -',/ &
    ' Message: Maximum number of particles in the system MAX_PIS', &
    /10X,' has been exceeded. Increase the value in mfix.dat',/ &
    1X,70('*')//)

RETURN
END SUBROUTINE DES_MASS_INLET

```

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! ~~~~~!
! Module name: DES_PLACE_NEW_PARTICLE!
! !
! Purpose: This routine uses the classification information to place !
! a new particle in the proper location. !
! !
! Author: J.Musser ! Date: 14-Aug-09 !
! !
! Comments: !
! !
! ~~~~~!

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        CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
    ENDDO
ENDIF
IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
    CALL RANDOM_NUMBER(RAND1)
    MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
    MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
        MI_WINDOW(BCV_I)
    DES_POS_OLD(NP,2) = RAND1 *&
        (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room
    MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
        DES_BC_Y_s(BCV) !shift relative to BC location
    IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE))THEN
        MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
    ELSE
        MI_FACTOR(BCV_I) = 1
    ENDIF
ENDIF

! 2D domain with verticle mass inlet: (east face)
! -----
    CASE ('XE')
! Offset Y axis by 1 particle diameter into ghost cell
    DES_POS_OLD(NP,1) = XLENGTH + (DES_BC_OFFSET(BCV_I))

    IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
        DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
            CALL RANDOM_NUMBER(RAND1)
! Place randomly between DES_BC_Y_s(BCV) and DES_BC_Y_n(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
            DES_POS_OLD(NP,2) = DES_BC_Y_s(BCV) + DES_RADIUS(NP) +&
                RAND1*(DES_BC_Y_n(BCV)-DES_BC_Y_s(BCV) -&
                2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
            CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
        ENDDO
    ENDIF
    IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
        CALL RANDOM_NUMBER(RAND1)
        MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
        MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
            MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,2) = RAND1 *&
            (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
            DES_BC_Y_s(BCV) !shift relative to BC location
        IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE))THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
        ELSE
            MI_FACTOR(BCV_I) = 1
        ENDIF
    ENDIF

! 2D domain with horizontal mass inlet: (south face)
! -----
    CASE ('YS')
! Offset X axis by 1 particle diameter into ghost cell

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DES_POS_OLD(NP,2) = -(DES_BC_OFFSET(BCV_I))

IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
  DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
    CALL RANDOM_NUMBER(RAND1)
! Place randomly between DES_BC_X_w(BCV) and DES_BC_X_e(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
    DES_POS_OLD(NP,1) = DES_BC_X_w(BCV) + DES_RADIUS(NP) +&
      RAND1*(DES_BC_X_e(BCV) - DES_BC_X_w(BCV) -&
        2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
    CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
  ENDDO
ENDIF
IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
  CALL RANDOM_NUMBER(RAND1)
  MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
  MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
    MI_WINDOW(BCV_I)
  DES_POS_OLD(NP,1) = RAND1 *&
    (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room
  MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
  DES_BC_X_w(BCV) !shift relative to BC location
  IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE))THEN
    MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
  ELSE
    MI_FACTOR(BCV_I) = 1
  ENDIF
ENDIF

! 2D domain with horizontal mass inlet: (north face)
! -----
CASE ('YN')
! Offset X axis by 1 particle diameter into ghost cell
  DES_POS_OLD(NP,2) = YLENGTH + (DES_BC_OFFSET(BCV_I))

  IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
    DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
      CALL RANDOM_NUMBER(RAND1)
! Place randomly between DES_BC_X_w(BCV) and DES_BC_X_e(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
      DES_POS_OLD(NP,1) = DES_BC_X_w(BCV) + DES_RADIUS(NP) +&
        RAND1*(DES_BC_X_e(BCV) - DES_BC_X_w(BCV) -&
          2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
      CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
    ENDDO
  ENDIF
  IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
    CALL RANDOM_NUMBER(RAND1)
    MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
    MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
      MI_WINDOW(BCV_I)
    DES_POS_OLD(NP,1) = RAND1 *&
      (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) + & !play room

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```

        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&    !shift loc. into
window
        DES_BC_X_w(BCV)    !shift relative to BC location
        IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE)) THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
        ELSE
            MI_FACTOR(BCV_I) = 1
        ENDIF
    ENDIF

! 3D domain with mass inlet on XZ plane: (south face)
! -----
        CASE ('XZs')
! Offset XZ plane by 1 particle diameter into ghost cell
        DES_POS_OLD(NP,2) = -(DES_BC_OFFSET(BCV_I))
        IF(PARTICLE_PLCMNT(BCV_I) == 'RAND') THEN
            DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
                CALL RANDOM_NUMBER(RAND1)
                CALL RANDOM_NUMBER(RAND2)
! Place randomly between DES_BC_X_w(BCV) and DES_BC_X_e(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
                DES_POS_OLD(NP,1) = DES_BC_X_w(BCV) + DES_RADIUS(NP) +&
                    RAND1*(DES_BC_X_e(BCV) - DES_BC_X_w(BCV) -&
                        2.0d0*DES_RADIUS(NP))
! Place randomly between DES_BC_Z_b(BCV) and DES_BC_Z_t(BCV)
                DES_POS_OLD(NP,3) = DES_BC_Z_b(BCV) + DES_RADIUS(NP) +&
                    RAND2*(DES_BC_Z_t(BCV) - DES_BC_Z_b(BCV) -&
                        2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
                CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
            ENDDO
        ENDIF
        IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR') THEN
! Obtain a random number from (0,1]
            CALL RANDOM_NUMBER(RAND1)
            CALL RANDOM_NUMBER(RAND2)
! Determine x-coordinate from ordered grid position I
            MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
            MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
                MI_WINDOW(BCV_I)
            DES_POS_OLD(NP,1) = RAND1 *&
                (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&    !play room
            MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&    !shift loc. into
window
            DES_BC_X_w(BCV)    !shift relative to BC location
! Determine z-coordinate from ordered grid position J
            MI_WIN = dble(J_OF_MI(BCV_I)%VALUE(MI_ORD))*&
                MI_WINDOW(BCV_I)
            DES_POS_OLD(NP,3) = RAND2 *&
                (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&    !play room
            MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&    !shift loc. into
window
            DES_BC_Z_b(BCV)    !shift relative to BC location
! Increment MI_FACTOR by one or loop back to one
            IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE)) THEN
                MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
            ELSE
                MI_FACTOR(BCV_I) = 1
            ENDIF
        ENDIF
    ENDIF

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```

! 3D domain with mass inlet on XZ plane: (north face)
! -----
      CASE ('XZn')
! Offset XZ plane by 1 particle diameter into ghost cell
      DES_POS_OLD(NP,2) = YLENGTH + (DES_BC_OFFSET(BCV_I))
      IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
        DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
          CALL RANDOM_NUMBER(RAND1)
          CALL RANDOM_NUMBER(RAND2)
! Place randomly between DES_BC_X_w(BCV) and DES_BC_X_e(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
          DES_POS_OLD(NP,1) = DES_BC_X_w(BCV) + DES_RADIUS(NP) +&
            RAND1*(DES_BC_X_e(BCV) - DES_BC_X_w(BCV) -&
              2.0d0*DES_RADIUS(NP))
! Place randomly between DES_BC_Z_b(BCV) and DES_BC_Z_t(BCV)
          DES_POS_OLD(NP,3) = DES_BC_Z_b(BCV) + DES_RADIUS(NP) +&
            RAND2*(DES_BC_Z_t(BCV) - DES_BC_Z_b(BCV) -&
              2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
          CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
        ENDDO
      ENDIF
      IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
          CALL RANDOM_NUMBER(RAND1)
          CALL RANDOM_NUMBER(RAND2)
          MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
! Determine x-coordinate from ordered grid position I
          MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
            MI_WINDOW(BCV_I)
          DES_POS_OLD(NP,1) = RAND1 *&
            (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&      !play room
            MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&      !shift loc. into
window
          DES_BC_X_w(BCV)      !shift relative to BC location
! Determine z-coordinate from ordered grid position J
          MI_WIN = dble(J_OF_MI(BCV_I)%VALUE(MI_ORD))*&
            MI_WINDOW(BCV_I)
          DES_POS_OLD(NP,3) = RAND2 *&
            (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&      !play room
            MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&      !shift loc. into
window
          DES_BC_Z_b(BCV)      !shift relative to BC location
! Increment MI_FACTOR by one or loop back to one
          IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE))THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
          ELSE
            MI_FACTOR(BCV_I) = 1
          ENDIF
        ENDIF
      ENDIF

! 3D domain with mass inlet on XY plane: (bottom face)
! -----
      CASE ('XYb')
! Offset XY plane by 1 particle diameter into ghost cell
      DES_POS_OLD(NP,3) = -(DES_BC_OFFSET(BCV_I))

      IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
        DO WHILE (TOUCHING)
! Obtain a random number from (0,1]

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        CALL RANDOM_NUMBER(RAND1)
        CALL RANDOM_NUMBER(RAND2)
! Place randomly between DES_BC_X_w(BCV) and DES_BC_X_e(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
        DES_POS_OLD(NP,1) = DES_BC_X_w(BCV) + DES_RADIUS(NP) +&
        RAND1*(DES_BC_X_e(BCV) - DES_BC_X_w(BCV) -&
        2.0d0*DES_RADIUS(NP))
! Place randomly between DES_BC_Y_s(BCV) and DES_BC_Y_n(BCV)
        DES_POS_OLD(NP,2) = DES_BC_Y_s(BCV) + DES_RADIUS(NP) +&
        RAND2*(DES_BC_Y_n(BCV) - DES_BC_Y_s(BCV) -&
        2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
        CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
        ENDDO
    ENDIF
    IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
        CALL RANDOM_NUMBER(RAND1)
        CALL RANDOM_NUMBER(RAND2)
        MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
! Determine x-coordinate from ordered grid position I
        MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
        MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,1) = RAND1 *&
        (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&      !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&      !shift loc. into
window
        DES_BC_X_w(BCV)      !shift relative to BC location
! Determine y-coordinate from ordered grid position J
        MI_WIN = dble(J_OF_MI(BCV_I)%VALUE(MI_ORD))*&
        MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,2) = RAND2 *&
        (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&      !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&      !shift loc. into
window
        DES_BC_Y_s(BCV)      !shift relative to BC location
! Increment MI_FACTOR by one or loop back to one
        IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE))THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
        ELSE
            MI_FACTOR(BCV_I) = 1
        ENDIF
    ENDIF

! 3D domain with mass inlet on XY plane: (top face)
! -----
        CASE ('XYt')
! Offset XY plane by 1 particle diameter into ghost cell
        DES_POS_OLD(NP,3) = ZLENGTH + (DES_BC_OFFSET(BCV_I))

        IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
            DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
                CALL RANDOM_NUMBER(RAND1)
                CALL RANDOM_NUMBER(RAND2)
! Place randomly between DES_BC_X_w(BCV) and DES_BC_X_e(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
                DES_POS_OLD(NP,1) = DES_BC_X_w(BCV) + DES_RADIUS(NP) +&
                RAND1*(DES_BC_X_e(BCV) - DES_BC_X_w(BCV) -&
                2.0d0*DES_RADIUS(NP))
! Place randomly between DES_BC_Y_s(BCV) and DES_BC_Y_n(BCV)

```

```

        DES_POS_OLD(NP,2) = DES_BC_Y_s(BCV) + DES_RADIUS(NP) +&
        RAND2*(DES_BC_Y_n(BCV) - DES_BC_Y_s(BCV) -&
        2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
        CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
    ENDDO
ENDIF
    IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]
        CALL RANDOM_NUMBER(RAND1)
        CALL RANDOM_NUMBER(RAND2)
        MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
! Determine x-coordinate from ordered grid position I
        MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
        MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,1) = RAND1 *&
        (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
        DES_BC_X_w(BCV) !shift relative to BC location
! Determine y-coordinate from ordered grid position J
        MI_WIN = dble(J_OF_MI(BCV_I)%VALUE(MI_ORD))*&
        MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,2) = RAND2 *&
        (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
        DES_BC_Y_s(BCV) !shift relative to BC location
! Increment MI_FACTOR by one or loop back to one
        IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE))THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
        ELSE
            MI_FACTOR(BCV_I) = 1
        ENDIF
    ENDIF

! 3D domain with mass inlet on YZ plane: (west face)
! -----
    CASE ('YZw')
! Offset YZ plane by 1 particle diameter into ghost cell
        DES_POS_OLD(NP,1) = -(DES_BC_OFFSET(BCV_I))

        IF(PARTICLE_PLCMNT(BCV_I) == 'RAND')THEN
            DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
                CALL RANDOM_NUMBER(RAND1)
                CALL RANDOM_NUMBER(RAND2)
! Place randomly between DES_BC_Y_s(BCV) and DES_BC_Y_n(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
                DES_POS_OLD(NP,2) = DES_BC_Y_s(BCV) + DES_RADIUS(NP) +&
                RAND1*(DES_BC_Y_n(BCV) - DES_BC_Y_s(BCV) -&
                2.0d0*DES_RADIUS(NP))
! Place randomly between DES_BC_Z_b(BCV) and DES_BC_Z_t(BCV)
                DES_POS_OLD(NP,3) = DES_BC_Z_b(BCV) + DES_RADIUS(NP) +&
                RAND2*(DES_BC_Z_t(BCV) - DES_BC_Z_b(BCV) -&
                2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
                CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
            ENDDO
        ENDIF
        IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR')THEN
! Obtain a random number from (0,1]

```

```

        CALL RANDOM_NUMBER(RAND1)
        CALL RANDOM_NUMBER(RAND2)
        MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
! Determine y-coordinate from ordered grid position I
        MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
            MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,2) = RAND1 *&
            (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
        DES_BC_Y_s(BCV) !shift relative to BC location
! Determine z-coordinate from ordered grid position J
        MI_WIN = dble(J_OF_MI(BCV_I)%VALUE(MI_ORD))*&
            MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,3) = RAND2 *&
            (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) + & !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +& !shift loc. into
window
        DES_BC_Z_b(BCV) !shift relative to BC location
! Increment MI_FACTOR by one or loop back to one
        IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE)) THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
        ELSE
            MI_FACTOR(BCV_I) = 1
        ENDIF
    ENDIF

! 3D domain with mass inlet on YZ plane: (east face)
! -----
        CASE ('YZe')
! Offset YZ plane by 1 particle diameter into ghost cell
        DES_POS_OLD(NP,1) = XLENGTH + (DES_BC_OFFSET(BCV_I))

        IF(PARTICLE_PLCMNT(BCV_I) == 'RAND') THEN
            DO WHILE (TOUCHING)
! Obtain a random number from (0,1]
                CALL RANDOM_NUMBER(RAND1)
                CALL RANDOM_NUMBER(RAND2)
! Place randomly between DES_BC_Y_s(BCV) and DES_BC_Y_n(BCV) and ensure
! that the particle center will be placed a radius away from either edge
! of the inlet
                DES_POS_OLD(NP,2) = DES_BC_Y_s(BCV) + DES_RADIUS(NP) +&
                    RAND1*(DES_BC_Y_n(BCV) - DES_BC_Y_s(BCV) -&
                    2.0d0*DES_RADIUS(NP))
! Place randomly between DES_BC_Z_b(BCV) and DES_BC_Z_t(BCV)
                DES_POS_OLD(NP,3) = DES_BC_Z_b(BCV) + DES_RADIUS(NP) +&
                    RAND2*(DES_BC_Z_t(BCV) - DES_BC_Z_b(BCV) -&
                    2.0d0*DES_RADIUS(NP))
! Test that no new particles are touching
                CALL DES_NEW_PARTICLE_TEST(NP, BCV_I, TOUCHING)
            ENDDO
        ENDIF
        IF(PARTICLE_PLCMNT(BCV_I) == 'ORDR') THEN
! Obtain a random number from (0,1]
            CALL RANDOM_NUMBER(RAND1)
            CALL RANDOM_NUMBER(RAND2)
            MI_ORD = MI_ORDER(BCV_I)%VALUE(MI_FACTOR(BCV_I))
! Determine y-coordinate from ordered grid position I
            MI_WIN = dble(I_OF_MI(BCV_I)%VALUE(MI_ORD))*&
                MI_WINDOW(BCV_I)
            DES_POS_OLD(NP,2) = RAND1 *&
                (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +& !play room

```

```

        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&    !shift loc. into
window
        DES_BC_Y_s(BCV)    !shift relative to BC location
! Determine z-coordinate from ordered grid position J
        MI_WIN = dble(J_OF_MI(BCV_I)%VALUE(MI_ORD))*&
        MI_WINDOW(BCV_I)
        DES_POS_OLD(NP,3) = RAND2 * &
        (MI_WINDOW(BCV_I) - (DES_RADIUS(NP)*2.0d0)) +&    !play room
        MI_WIN + (DES_RADIUS(NP)*2.0d0)*HALF +&    !shift loc. into
window
        DES_BC_Z_b(BCV)    !shift relative to BC location
! Increment MI_FACTOR by one or loop back to one
        IF(MI_FACTOR(BCV_I) < SIZE(MI_ORDER(BCV_I)%VALUE)) THEN
            MI_FACTOR(BCV_I) = MI_FACTOR(BCV_I) + 1
        ELSE
            MI_FACTOR(BCV_I) = 1
        ENDIF
    ENDIF

    CASE DEFAULT
        PRINT*, 'INVALID DES MASS INLET CLASSIFICATION'
        CALL MFIX_EXIT(myPE)
    END SELECT

RETURN
END SUBROUTINE DES_PLACE_NEW_PARTICLE

```



```

! ~~~~~
!
! Module name:  DES_NEW_PARTICLE_TEST
!
! Purpose:  This routine checks if a new particle placed using the
! random inlet was placed in contact with an existing particle.  If
! so a flag is set indicating contact, and the new particle is
! repositioned within the inlet domain.
!
! Author:  J.Musser
!
! Date:  14-Aug-09
!
! Comments:
!
! ~~~~~

```

219

```

        DISTVEC(:) = DES_POS_OLD(NP,:) - DES_POS_NEW(NP2,:)
        DIST = SQRT(DES_DOTPRDCT(DISTVEC,DISTVEC))
        R_LM = DES_RADIUS(NP) + DES_RADIUS(NP2)
        IF(DIST .LE. R_LM) TOUCHING = .TRUE.
    ENDDO
ENDIF
ENDDO
ENDDO
ENDDO

RETURN
END SUBROUTINE DES_NEW_PARTICLE_TEST

```

```

! ~~~~~!
! Module name: DES_CHECK_PARTICLE!
!
! Purpose: This routine is used to check if a new particle has fully
! entered the domain. If so, the flag classifying the particle as new
! is removed, allowing the particle to respond to contact forces from
! walls and other particles.
!
!
! Author: J.Musser Date: 13-Jul-09!
!
! Comments:
! ~~~~~!
!
SUBROUTINE DES_CHECK_PARTICLE
!
USE compar
USE constant
USE des_bc
USE discretelement
USE funits
USE geometry
USE indices
USE param1
USE physprop
!
IMPLICIT NONE
!-----
! Local variables
!-----
      INTEGER I,J,K,IJK      ! Unused indices at this time
      INTEGER PC              ! Loop counter
      INTEGER NP              ! Particle Index
      INTEGER NPT             ! Temp Particle Index
! Tmp holder of particle position
      DOUBLE PRECISION XPOS, YPOS, ZPOS
!
! Loop indices used for clearing forces associated with exiting particles
      INTEGER NLIMNP, NLIM, NEIGHNP, NLIM_NEIGHNP
!
! Logical for local debug warnings
      LOGICAL DES_LOC_DEBUG
!-----
      INCLUDE 'function.inc'
!
      DES_LOC_DEBUG = .FALSE.
!
      PC = 1
      DO NP = 1, MAX_PIS
        IF(PC .GT. PIS) EXIT
        IF(.NOT.PEA(NP,1)) CYCLE
!
        XPOS = DES_POS_NEW(NP,1)
        YPOS = DES_POS_NEW(NP,2)
        IF (DIMN .EQ. 3) ZPOS = DES_POS_NEW(NP,3)
! check the status of a new injected particle. if the new particle
! fully entered the domain change its 'new' status PEA(NP,2) to false

```

```

      IF (PEA(NP,2)) THEN
        IF (DIMN == 2 .AND. &
          (XPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (XPOS + DES_RADIUS(NP)) .LT. XLENGTH.AND.&
          (YPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (YPOS + DES_RADIUS(NP)) .LT. YLENGTH &
        .OR. &
          DIMN == 3 .AND. &
          (XPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (XPOS + DES_RADIUS(NP)) .LT. XLENGTH.AND.&
          (YPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (YPOS + DES_RADIUS(NP)) .LT. YLENGTH .AND. &
          (ZPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (ZPOS + DES_RADIUS(NP)) .LT. ZLENGTH) THEN

          PEA(NP,2) = .FALSE.
          PC = PC + 1

        ENDIF ! end if particle has fully entered the system

! check the status of an exiting particle (a particle that has come into
! contact with a mass outlet).
      ELSEIF (PEA(NP,3)) THEN
        IF (DIMN == 2 .AND. &
          (XPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (XPOS + DES_RADIUS(NP)) .LT. XLENGTH.AND.&
          (YPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (YPOS + DES_RADIUS(NP)) .LT. YLENGTH &
        .OR. &
          DIMN == 3 .AND. &
          (XPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (XPOS + DES_RADIUS(NP)) .LT. XLENGTH.AND.&
          (YPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (YPOS + DES_RADIUS(NP)) .LT. YLENGTH .AND. &
          (ZPOS - DES_RADIUS(NP)) .GT. 0 .AND.&
          (ZPOS + DES_RADIUS(NP)) .LT. ZLENGTH) THEN
! if an exiting particle has altered course so that it is moving back
! into the domain change (no longer on track to exit the domain) and
! it has fully entered the domain then change its 'exiting' status
! PEA(NP,3) to false

          PEA(NP,3) = .FALSE.
          PC = PC + 1

        ELSEIF (DIMN == 2 .AND. &
          (XPOS + DES_RADIUS(NP)) .LE. 0 .OR.&
          (XPOS - DES_RADIUS(NP)) .GE. XLENGTH .OR.&
          (YPOS + DES_RADIUS(NP)) .LE. 0 .OR.&
          (YPOS - DES_RADIUS(NP)) .GT. YLENGTH &
        .OR. &
          DIMN == 3 .AND. &
          (XPOS + DES_RADIUS(NP)) .LE. 0 .OR.&
          (XPOS - DES_RADIUS(NP)) .GE. XLENGTH.OR.&
          (YPOS + DES_RADIUS(NP)) .LE. 0 .OR.&
          (YPOS - DES_RADIUS(NP)) .GE. YLENGTH .OR. &
          (ZPOS + DES_RADIUS(NP)) .LE. 0 .OR.&
          (ZPOS - DES_RADIUS(NP)) .GE. ZLENGTH) THEN
! if an exiting particle has fully exited the domain, effectively
! remove the particle (reset PEA(NP,:) to false)

          PEA(NP,:) = .FALSE.

          DES_POS_OLD(NP,:) = ZERO

```

```

DES_POS_NEW(NP,:) = ZERO
DES_VEL_OLD(NP,:) = ZERO
DES_VEL_NEW(NP,:) = ZERO
OMEGA_OLD(NP,:) = ZERO
OMEGA_NEW(NP,:) = ZERO
DES_RADIUS(NP) = ZERO
PMASS(NP) = ZERO
PVOL(NP) = ZERO
RO_Sol(NP) = ZERO
OMOI(NP) = ZERO

FC(NP,:) = ZERO
FN(NP,:) = ZERO
FT(NP,:) = ZERO
TOW(NP,:) = ZERO

PN(NP,:) = -1
PN(NP,1) = 0
PV(NP,:) = 1
PFT(NP,:,:) = ZERO
PPOS(NP,:) = ZERO

! Note that if particle NP has any neighbors then the particle NP will
! still exist in the neighbor's neighbours list. This information would
! eventually be cleared in the second call to calc_force_des following
! the removal of NP but is forceably removed here to keep the dem
! inlet/outlet code self contained (does not rely on other code)
NEIGHBOURS(NP,:) = -1
NEIGHBOURS(NP,1) = 0

! Clear particle NP from any other neighboring particles lists
IF (NEIGHBOURS(NP,1) > 0) THEN
    NLIMNP = NEIGHBOURS(NP,1)+1

! Cycle through all neighbours of particle NP
DO I = 2, NLIMNP
    NEIGHNP = NEIGHBOURS(NP,I)

! If any neighbor particle has a lower index than NP then the contact
! force history will be stored with that particle and needs to be cleared
IF (NEIGHNP < NP) THEN
    IF (PN(NEIGHNP,1) > 0) THEN
        NLIM = PN(NEIGHNP,1)+1
        DO J = 2, NLIM
            NPT = PN(NEIGHNP,J)
            IF (NPT .NE. NP) CYCLE ! find particle NP in
NEIGHNP list

            PN(NEIGHNP,J:(MAXNEIGHBORS-1)) = &
                PN(NEIGHNP,(J+1):MAXNEIGHBORS)
            PV(NEIGHNP,J:(MAXNEIGHBORS-1)) = &
                PV(NEIGHNP,(J+1):MAXNEIGHBORS)
            PFT(NEIGHNP,J:(MAXNEIGHBORS-1),:) = &
                PFT(NEIGHNP,(J+1):MAXNEIGHBORS,:)
            PN(NEIGHNP,1) = PN(NEIGHNP,1) -1
        ENDDO
    ENDIF
ENDIF

    NLIM_NEIGHNP = NEIGHBOURS(NEIGHNP,1)+1
! Find where particle NP is stored in its neighbours (NEIGHNP) lists
! and remove particle NP from the list
DO J = 2, NLIM_NEIGHNP
    NPT = NEIGHBOURS(NEIGHNP,J)

```

```

                                IF (NPT .NE. NP) CYCLE ! find particle NP in NEIGHNP
list
                                NEIGHBOURS (NEIGHNP,1) = NEIGHBOURS (NEIGHNP,1)-1
                                NEIGHBOURS (NEIGHNP,J: (MN-1)) =
NEIGHBOURS (NEIGHNP, (J+1):MN)
                                ENDDO
                                ENDDO
                                ENDIF

                                PIS = PIS - 1
! In the exiting case do not increment pc

                                ENDIF ! endif particle has reentered/exited of the domain

                                ELSE
                                PC = PC + 1
                                ENDIF ! endif PEA(NP,3) or PEA(NP,2)

                                ENDDO ! loop over NP=1,MAX_PIS

                                IF (DES_LOC_DEBUG) WRITE(*,1001)

1000 FORMAT(3X,'----- START DES_CHECK_PARTICLE ----->')
1001 FORMAT(3X,'<----- END DES_CHECK_PARTICLE -----')

! Can be used for debugging purposes
9000 FORMAT(F9.4,2X,'NOT NEW ',I4,1X,6(F9.4,1X))
9001 FORMAT(F9.4,2X,'RE-ENTER ',I4,1X,6(F9.4,1X))
9002 FORMAT(F9.4,2X,'EXITED ',I4)

                                RETURN
                                END SUBROUTINE DES_CHECK_PARTICLE

```

```

! ~~~~~
! Module name: DES_MASS_OUTLET(NP, BCC, WC)
!
! Purpose:
! Check if the particle's position overlaps the outlet position
! by more than its radius (i.e., the particle is more than just
! touching the boundary)
!
! Author: J.Musser                                Date: 5-Oct-09
!
! Comments:
!
! ~~~~~

SUBROUTINE DES_MASS_OUTLET(NP, BCC, WC)

  USE des_bc
  USE discretelement
  USE param1

  IMPLICIT NONE

!-----
! Local variables
!-----

  INTEGER NP          ! Particle ID Number
  INTEGER WC          ! Wall contact value (0: No Contact, 1: Contact)
  INTEGER BCV_I, BCV

  DOUBLE PRECISION XPOS, YPOS, ZPOS ! particle x,y,z position
  DOUBLE PRECISION RAD ! particle radius

  CHARACTER*2 BCC      ! Boundary condition class (Xw,Xe,Ys,Yn,Zb,Zt)

!-----

  RAD = DES_RADIUS(NP)

  XPOS = DES_POS_NEW(NP,1)
  YPOS = DES_POS_NEW(NP,2)
  IF (DIMN .EQ. 2) THEN
    ZPOS = ONE
  ELSE
    ZPOS = DES_POS_NEW(NP,3)
  ENDIF

! Set the flag identifying a wall contact to 1 (contact exists). If the
! particle is in contact with a region of the wall that is listed as an
! outlet for DES particles, then the wall contact is ignored by setting
! the flag back to zero.
  WC = 1

! Loop over all outflow boundary conditions
  DO BCV_I = 1, DES_BCMO
    BCV = DES_BC_MO_ID(BCV_I)
! Find which outlet boundary(s) index coincide with the passed boundary
! condition class.
    IF(DES_MO_CLASS(BCV_I) == BCC)THEN

```

```

      IF(DIMN == 2)THEN      ! 2D domain

        IF(BCC == 'XW' .OR. BCC == 'XE')THEN
          IF(DES_BC_Y_s(BCV) < (YPOS - RAD) .AND. &
             DES_BC_Y_n(BCV) > (YPOS + RAD) )THEN
            WC = 0
            PEA(NP,3) = .TRUE.
          ENDIF
        ENDIF
        IF(BCC == 'YS' .OR. BCC == 'YN' )THEN
          IF(DES_BC_X_w(BCV) < (XPOS - RAD) .AND. &
             DES_BC_X_e(BCV) > (XPOS + RAD) )THEN
            WC = 0
            PEA(NP,3) = .TRUE.
          ENDIF
        ENDIF

      ELSE ! 3D domain

        IF(BCC == 'XW' .OR. BCC == 'XE')THEN
          IF(DES_BC_Y_s(BCV) < (YPOS - RAD) .AND. &
             DES_BC_Y_n(BCV) > (YPOS + RAD) .AND. &
             DES_BC_Z_b(BCV) < (ZPOS - RAD) .AND. &
             DES_BC_Z_t(BCV) > (ZPOS + RAD) )THEN
            WC = 0
            PEA(NP,3) = .TRUE.
          ENDIF
        ENDIF
        IF(BCC == 'YS' .OR. BCC == 'YN')THEN
          IF(DES_BC_X_w(BCV) < (XPOS - RAD) .AND. &
             DES_BC_X_e(BCV) > (XPOS + RAD) .AND. &
             DES_BC_Z_b(BCV) < (ZPOS - RAD) .AND. &
             DES_BC_Z_t(BCV) > (ZPOS + RAD) )THEN
            WC = 0
            PEA(NP,3) = .TRUE.
          ENDIF
        ENDIF
        IF(BCC == 'ZB' .OR. BCC == 'ZT')THEN
          IF(DES_BC_X_w(BCV) < (XPOS - RAD) .AND. &
             DES_BC_X_e(BCV) > (XPOS + RAD) .AND. &
             DES_BC_Y_s(BCV) < (YPOS - RAD) .AND. &
             DES_BC_Y_n(BCV) > (YPOS + RAD) )THEN
            WC = 0
            PEA(NP,3) = .TRUE.
          ENDIF
        ENDIF

      ENDIF ! endif dimn == 2
    ENDIF ! endif DES_MO_CLASS(BCV_I) == BCC

  ENDDO ! loop over BCV_I the no. of outlet boundaries

9000 FORMAT(F9.4,2X,'PEA(3)=T ',I4,1X,6(F9.4,1X))

END SUBROUTINE DES_MASS_OUTLET

```


Appendix D: Particle heat transfer model source code

The section contains the source code for the particle heat transfer models. It has been written in the FORTRAN90/95 style.

D.1 Module – DES_IC

```

! ~~~~~
! Module name: DES_IC
!
! Purpose: Common elements needed for DES initial conditions.
!
!
! Author: J.Musser
!
! Date: 17-Feb-11
!
! Comments:
!
! ~~~~~
!
! MODULE DES_IC
!
! USE param
!
! Logical variable to determine whether an initial condition is defined
! LOGICAL DES_IC_DEFINED (DIMENSION_IC)
!
! Set to true if any DES initial condition regions are specified. This
! logical is used to invoke the call to DES_SET_IC.
! LOGICAL DES_IC_EXIST
!
! Physical coordinates indicating initial condition region
! DOUBLE PRECISION DES_IC_X_w(DIMENSION_IC)
! DOUBLE PRECISION DES_IC_X_e(DIMENSION_IC)
! DOUBLE PRECISION DES_IC_Y_s(DIMENSION_IC)
! DOUBLE PRECISION DES_IC_Y_n(DIMENSION_IC)
! DOUBLE PRECISION DES_IC_Z_b(DIMENSION_IC)
! DOUBLE PRECISION DES_IC_Z_t(DIMENSION_IC)
!
! Initial solids phase temperature in a specified region
! DOUBLE PRECISION DES_IC_T_s (DIMENSION_IC, DIM_M)
!
! Initial solids species mass fractions in a specified region
! DOUBLE PRECISION DES_IC_X_s (DIMENSION_IC, DIM_M, DIM_N_s)
!
! Density of unreacted, shrinking core
! DOUBLE PRECISION DES_IC_CORE_Rho(DIMENSION_IC, DIM_M)
!
! END MODULE DES_IC

```

```

! Module name: CHECK_DES_IC
! Purpose: Check the data provided for des initial conditions.
! Author: J.Musser Date: 17-Feb-11
! Comments:
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
SUBROUTINE CHECK_DES_IC

USE des_ic
USE discretelement
USE param
USE param1
USE des_thermo
USE des_rxns
USE compar
USE constant
USE funits
USE geometry
USE indices
USE physprop
USE run

IMPLICIT NONE

INTEGER ICV

!-----
! External functions
!-----

LOGICAL , EXTERNAL :: COMPARE

!-----

WRITE(*,'(1X,A)') '----- START CHECK_DES_IC ----->'

! Initialize the initial condition logical.
DES_IC_EXIST = .FALSE.

! Check for des inlet/outlet information:
CHECK IC: DO ICV = 1, DIMENSION_IC
    DES_IC_DEFINED(ICV) = .FALSE.
    IF (DES_IC_X_w(ICV) /= UNDEFINED) DES_IC_DEFINED(ICV) = .TRUE.
    IF (DES_IC_X_e(ICV) /= UNDEFINED) DES_IC_DEFINED(ICV) = .TRUE.
    IF (DES_IC_Y_s(ICV) /= UNDEFINED) DES_IC_DEFINED(ICV) = .TRUE.
    IF (DES_IC_Y_n(ICV) /= UNDEFINED) DES_IC_DEFINED(ICV) = .TRUE.
    IF (DES_IC_Z_b(ICV) /= UNDEFINED) DES_IC_DEFINED(ICV) = .TRUE.
    IF (DES_IC_Z_t(ICV) /= UNDEFINED) DES_IC_DEFINED(ICV) = .TRUE.

! If an initial condition is specified, verify necessary data
! Check that all dimensions have been defined
IF (DES_IC_DEFINED(ICV)) THEN
    IF (DES_IC_X_w(ICV) == UNDEFINED .OR. &
        DES_IC_X_e(ICV) == UNDEFINED .OR. &

```

```

        DES_IC_Y_s(ICV) == UNDEFINED .OR. &
        DES_IC_Y_n(ICV) == UNDEFINED) THEN
        WRITE (UNIT_LOG, 1000) ICV
        WRITE (*, 1000) ICV
        CALL MFIX_EXIT(myPE)
    ENDIF
    IF(DIMN == 3) THEN
        IF(DES_IC_Z_b(ICV) == UNDEFINED .OR. &
           DES_IC_Z_t(ICV) == UNDEFINED) THEN
            WRITE (UNIT_LOG, 1000) ICV
            WRITE (*, 1000) ICV
            CALL MFIX_EXIT(myPE)
        ENDIF
    ENDIF
! Check that the region does not overlap
    IF(DES_IC_X_w(ICV) .LT. ZERO .OR. &
       DES_IC_Y_s(ICV) .LT. ZERO .OR. &
       DES_IC_X_e(ICV) .GT. XLENGTH .OR. &
       DES_IC_Y_n(ICV) .GT. YLENGTH .OR. &
       DES_IC_X_w(ICV) .GT. DES_IC_X_e(ICV) .OR. &
       DES_IC_Y_s(ICV) .GT. DES_IC_Y_n(ICV)) THEN
        WRITE (UNIT_LOG, 1001) ICV
        WRITE (*, 1001) ICV
        CALL MFIX_EXIT(myPE)
    ENDIF

    IF(DIMN == 3) THEN
        IF(DES_IC_Z_b(ICV) .LT. 0 .OR. &
           DES_IC_Z_t(ICV) .GT. ZLENGTH .OR. &
           DES_IC_Z_b(ICV) .GT. DES_IC_Z_t(ICV)) THEN
            WRITE (UNIT_LOG, 1001) ICV
            WRITE (*, 1001) ICV
            CALL MFIX_EXIT(myPE)
        ENDIF
    ENDIF

! This is used to invoke the call to DES_SET_IC which is only done
! if there are valid initial conditions specified.
    DES_IC_EXIST = .TRUE.

    ENDIF ! end if DES_IC_DEFINED(ICV)

ENDDO CHECK_IC

! If the DES energy equations or DES species equation are being solve
! then initial conditions must be specified to provide the initial
! state of the particles.
    IF(.NOT.DES_IC_EXIST) THEN
        IF(DES_ENERGY_EQ) THEN
            WRITE(*,1002)'temperature','energy equation'
            WRITE(UNIT_LOG,1002)
            CALL MFIX_EXIT(myPE)
        ELSEIF(ANY_DES_SPECIES_EQ) THEN
            WRITE(*,1002)'species mass fractions','species equation'
            WRITE(UNIT_LOG,1002)
            CALL MFIX_EXIT(myPE)
        ENDIF
    ENDIF

    WRITE(*, '(1X,A)') '<----- END CHECK_DES_IC -----'

1000 FORMAT(/1X,70('*')/, ' From: CHECK_DES_IC',/, ' Message: ',&

```

```

        'Insufficient DEM initial condition infomation',/10X,&
        'Check initial condition number: ',I3,/1X,70('*')/)

1001 FORMAT(/1X,70('*')/, ' From: CHECK_DES_IC',/, ' Message: ',&
        'Improper DEM initial condition information',/10X,&
        'Check initial condition number: ',I3,/1X,70('*')/)

1002 FORMAT(/1X,70('*')/, ' From: CHECK_DES_IC',/'Message: Initial',    &
        ' condition data specifying the paritcle',/A,' is requied',    &
        ' when solving the ',A,'.',/' Check mfix.dat.',/1X,70('*')/)

RETURN
END SUBROUTINE CHECK_DES_IC

```

[illegible]

```

                Z_POS .LE. DES_IC_Z_T(ICV)) ) THEN
            ENDIF
! Change the flag to indicate that an IC region has been found.
            IC_FOUND = .TRUE.
! Exit the loop and assign the initial conditions to particle I.
            EXIT
        ENDIF
    ENDIF
ENDDO

    IF(IC_FOUND) THEN
! Assign the initial values for the specified models.
        CALL SET_DES_TEMPERATURE(I,ICV,M)
        CALL SET_DES_MASS_FRACTION(I,ICV,M)
        CALL SET_DES_CORE_DENSITY(I,ICV,M)
    ELSE
        IF(DIMN == 2) Z_POS = 0.0d0
        WRITE(*,1000)I, X_POS, Y_POS, Z_POS
        WRITE(UNIT_LOG,1000)I, X_POS, Y_POS, Z_POS
        CALL MFIX_EXIT(myPE)
    ENDIF
! increment the particle counter
    PC = PC + 1
ENDDO

1000 FORMAT(/1X,70('*')/, ' From: SET_DES_IC',/, ' Message:',      &
           ' There is no initial condition associated with the region',/ &
           ' containing particle ',I6,',',/, ' X Position: ',F9.4, /    &
           ' Y Position: ',F9.4,/' Z Position: ',F9.4,/' Please check', &
           ' the mfix.dat file.',/                                     &
           1X,70('*')/)

CONTAINS

!.....!
! Subroutine: SET_DES_TEMPERATURE                                     !
!.....!
! Purpose: Set the initial temperature of a partile.                 !
!.....!
    SUBROUTINE SET_DES_TEMPERATURE(I,ICV,M)
    INTEGER, INTENT(IN) :: I, ICV, M

! Initial temperatures must be specified for particles when solving
! the internal energy equation and species equation for a particle.
    IF(.NOT.ANY_DES_SPECIES_EQ .AND. .NOT.DES_ENERGY_EQ ) RETURN

    IF(DEG_IC_T_s(ICV,M) == UNDEFINED) THEN
        WRITE(*,1000)ICV,M,I
        WRITE(UNIT_LOG,1000)ICV,M,I
        CALL MFIX_EXIT(myPE)
    ELSE
        DES_T_s_NEW(I) = DEG_IC_T_s(ICV,M)
    ENDIF

! Set the value of the old temperature to the initial value.
    DES_T_s_OLD(I) = DES_T_s_NEW(I)

    RETURN

1000 FORMAT(/1X,70('*')/, ' From: SET_DES_IC',/, ' Message: The',      &
           ' initial temperature is UNDEFINED for particle ',I6,',',/    &
           ' This is required when solving the internal energy equation',&
           ' and species',/' equation for a particle. Check mfix.dat', &

```

```

        ' file.',/1X,70('*')/)

END SUBROUTINE SET_DES_TEMPERATURE

! .....!
! Subroutine: SET_DES_MASS_FRAC                                !
! .....!
! Purpose: Set the initial species mass fraction of a partile. !
! .....!
SUBROUTINE SET_DES_MASS_FRACTION(I,ICV,M)
  INTEGER, INTENT(IN) :: I, ICV, M

  INTEGER N ! species loop index

  DOUBLE PRECISION SUM

! The initial species mass fractions for a particle must be supplied if
! the species equation is being solved or if DES_C_PS0 has not been
! specified in conjunction with the energy equations being solved.
  IF(.NOT.ANY_DES_SPECIES_EQ .AND. (.NOT.DES_ENERGY_EQ .OR. &
    (DES_ENERGY_EQ .AND. DES_C_PS0(M) /= UNDEFINED) ) ) RETURN

! Verify that the species mass fraction sums to one.
  SUM = ZERO
  DO N=1,DES_NMAX(M)
    IF(DES_IC_X_s(ICV,M,N) /= UNDEFINED) THEN
      DES_X_s(I,N) = DES_IC_X_s(ICV,M,N)
      SUM = SUM + DES_IC_X_s(ICV,M,N)
    ELSE
      DES_X_s(I,N) = ZERO
    ENDIF
  ENDDO
  IF(.NOT.COMPARE(ONE,SUM)) THEN
    WRITE(*,1000) I
    WRITE(UNIT_LOG,1000) I
    CALL MFIX_EXIT(myPE)
  ENDIF

  RETURN

1000 FORMAT(/1X,70('*')/, ' From: SET_DES_IC',/, ' Message: The',      &
  ' species mass fraction of particle ',I6,' does not sum',/      &
  ' to one. This is required if solving the discrete particle', &
  ' species',/' equation or if DES_C_PS0 is not specified when',&
  ' solving the internal',/' energy equation for a particle.', &
  ' Check mfix.dat file.',/1X,70('*')/)

END SUBROUTINE SET_DES_MASS_FRACTION

! .....!
! Subroutine: SET_DES_CORE_DENSITY                                !
! .....!
! Purpose: Set the density of shrinking, unreacted core of a partile. !
! .....!
SUBROUTINE SET_DES_CORE_DENSITY(I,ICV,M)
  INTEGER, INTENT(IN) :: I, ICV, M

! Error indicating that an error has been specified to the user.
  LOGICAL, SAVE :: WARNED = .FALSE.

! Set the density of the unreacted core for reactive gas-solid flows.
! This value is *optional* but effects how the radius of the core
! changes during a reaction. If a value is not provided in the mfix.dat

```

```

! file, the density of the particle is assigned to the core.
  IF(.NOT.DES_SPECIES_EQ(M) .OR. TRIM(REACTION_MODEL) /= &
    'SHRINKING_CORE') RETURN

  IF(DES_IC_CORE_Rho(ICV,M) == UNDEFINED) THEN
    IF(.NOT.WARNED) THEN
      WRITE(*,1000)
      WRITE(UNIT_LOG,1000)
      WARNED = .TRUE.
    ENDIF
    CORE_Rho(I) = RO_Sol(I)
  ELSE
    CORE_Rho(I) = DES_IC_CORE_Rho(ICV,M)
  ENDIF

  RETURN

1000 FORMAT(/1X,70('*')/, ' From: SET_DES_IC',/, ' Message: Some or', &
  ' all of the discrete solids phases do not have an',/ &
  ' initial core density defined. This effects how the', &
  ' shrinking',/, ' unreacted core model behaves.',/, ' The', &
  ' core density will be set to the particle density.',/, &
  1X,70('*')/)

END SUBROUTINE SET_DES_CORE_DENSITY

END SUBROUTINE DES_SET_IC

```



```

! ~~~~~!
! Module name: DES_THERMO !
! !
! Purpose: Common elements for MFIX-DEM heat transfer. !
! condition. !
! !
! Author: J.Musser Date: 16-Jun-10 !
! !
! Comments: !
! !
! ^^^^^^!
MODULE DES_THERMO
USE param

! Run time logicals
!-----
! Slove DES Energy Equations
LOGICAL DES_ENERGY_EQ

! Specifies that the convection model is to be solved.
! Requires DES_ENERGY_EQ = .TRUE.
! Default [.TRUE.]
LOGICAL DES_CONV_EQ
! Specifies that the particle conduction models are to be solved.
! Requires DES_ENERGY_EQ = .TRUE.
! Default [.TRUE.]
LOGICAL DES_COND_EQ
! These logicals can be set in the mfix.dat file to omit specific
! particle-particle heat conduction models from being solved.
! If the DEM conduction model is not solved (DES_COND_EQ), the values
! are automatically set to .FALSE. in check_des_thermo.f.
! Default [.TRUE.]
LOGICAL DES_COND_EQ_PFP ! particle-fluid-particle
! Default [.TRUE.]
LOGICAL DES_COND_EQ_PP ! particle-particle
! Specifies that the particle-environment radiation model is to be
! solved. Requires DES_ENERGY_EQ = .TRUE.
! Default [.TRUE.]
LOGICAL DES_RADI_EQ

! Heat transfer correlation specified in mfix.dat
! Default [RANZ_1952]
CHARACTER*24 :: DES_CONV_CORR

! Specifies that a thermodynamic neighborhood for a particle be
! determined. This neighborhood can be much larger than the one
! established for determining collisions. It is used in conduction and
! radiation models.
LOGICAL FIND_THERMO_NBRHD

! Particle properties
!-----
! Particle temperature at current time step (S_TIME)
DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DES_T_s_OLD !(PARTICLES)
! Particle temperature at previous time step (S_TIME - DT_SOLID)
DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DES_T_s_NEW !(PARTICLES)

```

```

! DES Specified constant solids thermal conductivity by solids phase
  DOUBLE PRECISION DES_K_s0(DIM_M)
! DES solids thermal conductivity by particle ! (not currently used)
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DES_K_s

! DES Specified constant solids specific heat by solids phase
  DOUBLE PRECISION DES_C_ps0(DIM_M)
! DES specific heat of particles by particle
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: DES_C_ps

! Emissivity of particles
  DOUBLE PRECISION DES_Em(DIM_M)
! Stefan-Boltzmann Constant
  DOUBLE PRECISION SB_CONST

! Rates of heat transfer
!-----
! Heat transfer TO the particle from the fluid. This value will be positive
! when the particle is heating and negative when the particle is cooling.
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: Qcv !(PARTICLES)
! Heat transfer TO the particle from neighboring particles via the particle-
! particle conduction model. This value will be positive when the particle is
! heating and negative when the particle is cooling.
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: Qpp !(PARTICLES)
! Heat transfer TO the particle from neighboring particles via the particle-
! fluid-particle model. This value will be positive when the particle is
! heating and negative when the particle is cooling.
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: Qpfp !(PARTICLES)
! Heat transfer TO the particle from neighboring particles via radiation
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: Qrd !(PARTICLES)
! Internal heat generation resulting from a chemical reaction
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: Qint !(PARTICLES)
! Previous time step's rate of heat transfer. Used for Adams-Bashforth
! time integration scheme
  DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: Qtotal_OLD

! Thermodynamic Neighborhood
!-----
! Thermodynamic neighborhood. This is the list of particles around a
! particle that may transfer energy with the given particle.
  INTEGER, DIMENSION(:,:), ALLOCATABLE :: THERMO_NBRHD ! (PARTICLES,
MAXNEIGHBORS)
! This is the size of the thermodynamic neighborhood. Is is based on the
! maximum particle radius and the FLPC and RDPC
  DOUBLE PRECISION NBRHD_SZ
! Fluid Lens Proportion Constant used to calculate the radius of the
! fluid lens that surrounds the particle for particle-fluid-particle
! conduction. Default [ 0.2 ]
  DOUBLE PRECISION FLPC
! Radius of the radiation domain in relation of the particle diameter.
! Default [ 3.0 ] * DES_RADIUS(-)
  DOUBLE PRECISION RDPC
! Minimum separation distance between the surface of two contacting
! particles. This value is used to remove the singularity that the
! particle-fluid-particle conduction model develops at the contact
! interface. [4.0x10^(-10) meters]
  DOUBLE PRECISION DES_MIN_COND_DIST

END MODULE DES_THERMO

```

D.5 Routine – CHECK_DES_THERMO

```
! ~~~~~!  
! Module name: CHECK_DES_THERMO  
!  
! Purpose:  
!  
!  
! Author: J.Musser  
! Date: 17-Jun-10  
!  
! Comments:  
!  
! ~~~~~!  
  
      SUBROUTINE CHECK_DES_THERMO  
  
        Use compar  
        Use des_thermo  
        Use discretelement  
        Use funits  
        Use interpolation  
        Use physprop  
        Use run  
  
        IMPLICIT NONE  
  
!-----  
! Local variables  
!-----  
      INTEGER I, M ! dummy loop index  
  
! The size of the thermodynamic neighborhoods needed for particle-fluid-  
! particle conduction and radiation.  
      DOUBLE PRECISION SZ_PFP, SZ_RAD  
!-----  
! Functions  
!-----  
  
      WRITE(*,'(1X,A)') &  
          '----- START CHECK_DES_THERMO ----->'  
  
      IF(DEE_ENERGY_EQ) THEN  
  
! Loop over all solids phases  
      DO M=1,MMAK  
! Verify that the thermal conductivity values are physical.  
      IF(DEE_C_ps0(M) .LT. ZERO) THEN  
          WRITE(UNIT_LOG,1001)'DEE_K_s0','unphysical',M  
          WRITE(*,1001)'DEE_C_ps0','unphysical',M  
          CALL MFIX_EXIT(myPE)  
      ENDIF  
! Verify that the thermal conductivity values are physical and defined.  
      IF(DEE_K_s0(M) .LT. ZERO) THEN  
          WRITE(UNIT_LOG,1001)'DEE_K_s0','unphysical',M  
          WRITE(*,1001)'DEE_K_s0','unphysical',M  
          CALL MFIX_EXIT(myPE)  
      ELSEIF(DEE_K_s0(M) == UNDEFINED) THEN  
          WRITE(UNIT_LOG,1001)'DEE_K_s0','undefined',M  
          WRITE(*,1001)'DEE_K_s0','undefined',M  
          CALL MFIX_EXIT(myPE)  
      ENDIF  
    ENDDO
```

```

! Convection Equation:
! .....
      IF (DES_CONV_EQ) THEN
! Ensure that the continuum energy equations will be solved.
      IF (.NOT.ENERGY_EQ) THEN
        WRITE(*,1000)
        CALL MFIX_EXIT(myPE)
      ENDIF

      WRITE(*,'(6X,A)') 'DES convection model will be solved.'

      SELECT CASE (TRIM(DES_CONV_CORR))
! Verify the selected convective heat transfer coefficient model
      CASE ('RANZ_1952')
        ! Ranz, W.E. and Marshall, W.R., "Frication and transfer
        ! coefficients for single particles and packed beds,"
        ! Chemical Engineering Science, Vol. 48, No. 5, pp 247-253,
        ! 1925
! The Ranz and Marshall correlation needs no additional input from the
! user.
        WRITE(*,'(9X,A,A)') 'Heat transfer coefficient', &
          ' model: Ranz and Marshall (1952)'

! If the heat transfer coefficient correlation provided by the user does
! not match one of the models outlined above, flag the error and exit.
      CASE DEFAULT
        WRITE(*,'(6X,A)') &
          'INVALID DES CONVECTION MODEL (DES_CONV_CORR):'
        WRITE(*,'(6X,A)') 'The available models include:'
        WRITE(*,'(9X,A)') 'RANZ_1952 - Ranz and Marshall (1952)'
        CALL MFIX_EXIT
      END SELECT

    ELSE
      WRITE(*,'(6X,A)') 'DES convection model will NOT be solved.'
    ENDIF ! END convection model checks

! Conduction Equations:
! .....
      IF (DES_COND_EQ) THEN
        WRITE(*,'(6X,A)') 'DES conduction model will be solved.'

! Particle-particle Conduction:
! .....
        IF (DES_COND_EQ_PP) THEN
          DO M=1,MMAX
! Verify that a thermal conductivity value is specified for each solids
! phase and that the value is physical.
            IF (DES_K_S0(M) == UNDEFINED) THEN
              WRITE(UNIT_LOG,1001) 'DES_K_s0','undefined',M
              WRITE(*,1001) 'DES_K_s0','undefined',M
              CALL MFIX_EXIT(myPE)
            ELSEIF (DES_K_S0(M) .LT. ZERO) THEN
              WRITE(UNIT_LOG,1001) 'DES_K_s0','unphysical',M
              WRITE(*,1001) 'DES_K_s0','unphysical',M
              CALL MFIX_EXIT(myPE)
            ENDIF
          ENDDO
          WRITE(*,'(6X,A)') &
            'Solving the particle-particle conduction model.'
        ENDIF
      ENDIF

```

```

! A secondary neighborhood is established surrounding a particle to
! determine the neighboring particles for possible particle-particle
! heat transfer.
      FIND_THERMO_NBRHD = .TRUE.
    ELSE
      WRITE(*,'(5X,A)') &
        'NOT Solving the particle-particle conduction model.'
    ENDIF

! Particle-fluid-particle Conduction:
! .....
      IF(DS_COND_EQ_PFP) THEN
! Verify that either the simulation is coupled with a gas-phase
! simulation or that K_g0 has been provided in the dat file.
      IF(K_G0 == UNDEFINED .AND. &
        .NOT.DS_CONTINUUM_COUPLED) THEN
        WRITE(*,1002)
        WRITE(UNIT_LOG,1002)
        CALL MFX_EXIT(myPE)
      ENDIF

! Set the default value for the minimum distance separating particles'
! surfaces.
      IF(DS_MIN_COND_DIST == UNDEFINED) THEN
        DS_MIN_COND_DIST = 1.0D-04 ! cm
        IF (UNITS == 'SI') DS_MIN_COND_DIST = &
          DS_MIN_COND_DIST/100.0 ! m
      ENDIF

      WRITE(*,'(6X,A)') &
        'Solving the particle-fluid-particle conduction model.'
! A secondary neighborhood is established surrounding a particle to
! determine the neighboring particles for possible particle-fluid-
! particle heat transfer.
      FIND_THERMO_NBRHD = .TRUE.
    ELSE
      WRITE(*,'(6X,A)') &
        'NOT Solving the particle-fluid-particle conduction model.'
    ENDIF

    ELSE
      WRITE(*,'(6X,A)') 'DES conduction model will NOT be solved.'
! Set the logicals for the conduction sub-models to false.
! This should not be needed, but is done for precaution.
      DS_COND_EQ_PFP = .FALSE.
      DS_COND_EQ_PP = .FALSE.

    ENDIF ! END conduction model checks

! Radiation Equation:
! .....
      IF(DS_RADI_EQ) THEN
        WRITE(*,'(6X,A)') 'DES radiation model will be solved.'
! A secondary neighborhood is established surrounding a particle to
! determine the neighboring particles for possible radiative
! heat transfer.
        FIND_THERMO_NBRHD = .TRUE.
! Set the value of the Stefan-Boltzman Constant based on the units
        IF(UNITS == 'SI') THEN
!
          W/((m^2).K^4)
          SB_CONST = 5.6704d0*(10.0d0**(-8))
        ELSE
!
          cal/((cm^2).sec.K^4)

```

```

        SB_CONST = 1.355282d0*(10.0d0**(-12))
    ENDIF

    DO M=1,MMAX
! Verify that a emissivity value is specified for each solids pase
        IF(DES_Em(M) == UNDEFINED)THEN
            WRITE(UNIT_LOG,1001)'DES_Em','undefined',M
            WRITE(*,1001)'DES_Em','undefined',M
            CALL MFIX_EXIT(myPE)
        ELSEIF(DES_Em(M) .LT. ZERO .OR. &
            DES_Em(M) .GT. ONE) THEN
            WRITE(UNIT_LOG,1001)'DES_Em','unphysical',M
            WRITE(*,1001)'DES_Em','unphysical',M
            CALL MFIX_EXIT(myPE)
        ENDIF
    ENDDO
ELSE
    WRITE(*,'(6X,A)') 'DES radiation model will NOT be solved.'
ENDIF ! END radiation model checks

! Calculate the size of the thermodynamic neighbor (if needed)
IF( FIND_THERMO_NBRHD) THEN
    SZ_PFP = ZERO
! If solving conductive heat transfer, the minimum neighborhood size
! is [1.3]*DES_RADIUS by default. A buffer of 0.1 is added to ensure
! that the neighbor is seen as soon as possible. The size of the fluid
! lens for particle-fluid-particle heat transfer can be adjusted by
! specifying a different value in the mfix.dat file.
    IF(DES_COND_EQ_PP .OR. DES_COND_EQ_PFP) &
        SZ_PFP = MAX_RADIUS * ( 2.05d0 + FLPC )
    SZ_RAD = ZERO
! If radiation heat transfer is solved, the radius of the radiative
! heat transfer domain is [3.0]*DES_RADIUS by default. The size of the
! radiative heat transfer domain on the particle may be adjusted by
! specifying a new value in the mfix.dat file.
    IF(DES_RAD_EQ) &
        SZ_RAD = MAX_RADIUS * RDPC
    NBRHD_SZ = MAX( SZ_PFP, SZ_RAD )
    WRITE(*,'(6X,A,F10.6)') &
        'Radius of thermodynamic neighborhood is ',NBRHD_SZ
ENDIF ! FIND_THERMO_NBRHD

ELSE ! DES_ENERGY_EQ

    WRITE(*,'(6X,A)') 'DES energy equations are not being solved.'

! Reinitialize the heat transfer logicals to false.
    DES_CONV_EQ = .FALSE.
    DES_COND_EQ = .FALSE.
    DES_RAD_EQ = .FALSE.

    DES_COND_EQ_PFP = .FALSE.
    DES_COND_EQ_PP = .FALSE.

ENDIF ! DES_ENERGY_EQ

WRITE(*,'(1X,A)') &
    '<----- END CHECK_DES_THERMO -----'

RETURN

1000 FORMAT(/1X,70('*')/, ' From: CHECK_DES_THERMO',/, ' Message: ',&
    'The DES convection model requires that the energy ', &

```

```

        'equations',/1X,'(ENERGY_EQ) for the continuum phase must ',&
        'also be solved.',/1X,70('*')/)

1001 FORMAT(/1X,70('*')/, ' From: CHECK_DES_THERMO',/, ' Message: ',&
        A,' is ',A,' for solids phase ',I2,'. Check mfix.dat.', &
        /1X,70('*')/)

1002 FORMAT(/1X,70('*')/, ' From: CHECK_DES_THERMO',/, ' Message:',      &
        ' The particle-fluid-particle model requires that either a',      &
        ' simulation be coupled with a gas-phase simulation or that',      &
        ' K_g0 be',/, ' provided in the mfix.dat file. Check mfix.dat.', &
        /1X,70('*')/)

END SUBROUTINE CHECK_DES_THERMO

```

D.6 Routine – CALC_THERMO_DES

```

! Module name: CALC_THERMO_DES
! Purpose:
! Author: J.Musser Date: 16-Jun-10
! Comments:
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
      SUBROUTINE CALC_THERMO_DES(I, INTERP_IJK, INTERP_WEIGHTS, FOCUS)

        Use des_thermo
        Use discretelement
        Use fldvar
        Use interpolation
        Use paraml

        IMPLICIT NONE

! Passed variables
! -----
! Index of particle being looped over
    INTEGER, INTENT(IN) :: I
! IJK indicies of fluid cells involved in interpolation
    INTEGER, INTENT(IN) :: INTERP_IJK(INTERP_ORDER**DIMN)
! Weights associated with interpolation
    DOUBLE PRECISION, INTENT(IN) :: INTERP_WEIGHTS(INTERP_ORDER**DIMN)
! Indicates that debugging information for the particle
    LOGICAL, INTENT(IN) :: FOCUS

! Local variables
! -----
! Index of neighbor particle of particle I such that I < J
    INTEGER J
! Generic index of neighbor particle of particle I
    INTEGER JJ
! index to track accounted for particles
    INTEGER PC
! Number of particles in the radiation domain
    INTEGER N_RAD

! Distance between the centers of particle I and particle J (component)
    DOUBLE PRECISION DISTVEC(DIMN)
! Distance between the centers of particle I and particle J (magnitude)
    DOUBLE PRECISION CENTER_DIST
! Distance between the surfaces of particle I and particle J
    DOUBLE PRECISION SURFACE_DIST
! Angle generated between the line connecting the particle centers of
! particle I and J and the line generated by the center of particle I
! and one of the premiter of the circle generated by intersection area
! of particle I and particle J
    DOUBLE PRECISION ANG_IJ
! Radius of the circle created by the overlap of the spherical particles
    DOUBLE PRECISION R_sij
! Environment temperature used in the radiative heat transfer model
    DOUBLE PRECISION Ts RAD

```



```

! Functions
!-----
      DOUBLE PRECISION, EXTERNAL :: DES_DOTPRDCT

! calculate heat transfer via convection
      IF(DES_CONV_EQ) CALL DES_CONVECTION(I, INTERP_IJK, &
        INTERP_WEIGHTS, FOCUS)
! Loop over thermodynamic neighbor for conduction and radiation
      IF(DES_COND_EQ .OR. DES_RADI_EQ) THEN
! Initialize variables on entry
        Ts_RAD = ZERO
        N_RAD = 0
! Distance between particle centers
        IF (THERMO_NBRHD(I,1).GT.0) THEN
          DO JJ = 2, THERMO_NBRHD(I,1)+1
! Set the index of the neighbor particle
            J = THERMO_NBRHD(I,JJ)
! Skip the neighbor if it does not exist (should not be a problem)
            IF(.NOT.PEA(J,1) ) CYCLE
! Only do conduction calculations for particles with an index value
! higher than the current particle. The opposite heat transfer will be
! applied to the neighbor.
            IF(J.GT.I) THEN
! Calculate the center distance between the two particles
              DISTVEC(:) = DES_POS_NEW(I,:) - DES_POS_NEW(J,:)
              CENTER_DIST = SQRT(DES_DOTPRDCT(DISTVEC,DISTVEC))
! If the radiation heat transfer model is being solved, check to see
! if the particle J is within the domain of particle I.
              IF(DES_RADI_EQ) THEN
                IF(CENTER_DIST.LT.RDPC*DES_RADIUS(I)) THEN
! Increment the number of neighbors in the radiation domain and sum
! the temperature into the environment temperature (Ts_RAD)
                  N_RAD = N_RAD + 1
                  Ts_RAD = Ts_RAD + DES_T_s_NEW(J)
                ENDIF
              ENDIF
! Calculate particle-particle conduction
              IF(DES_COND_EQ) THEN
                CALL DES_CONDUCTION(I, J, CENTER_DIST, FOCUS)
              ENDIF
            ELSEIF(DES_RADI_EQ) THEN
! Calculate the center distance between the two particles
              DISTVEC(:) = DES_POS_NEW(I,:) - DES_POS_NEW(J,:)
              CENTER_DIST = SQRT(DES_DOTPRDCT(DISTVEC,DISTVEC))
! If the radiation heat transfer model is being solved, check to see
! if the particle J is within the domain of particle I.
              IF(RDPC*DES_RADIUS(I).GT.CENTER_DIST) THEN
! Increment the number of neighbors in the radiation domain and sum
! the temperature into the environment temperature (Ts_RAD)
                N_RAD = N_RAD + 1
                Ts_RAD = Ts_RAD + DES_T_s_NEW(J)
              ENDIF
            ENDIF ! J>I
          ENDDO ! Looping over neighbors
        ENDIF ! neighbors > 0
      ENDIF ! des_conduction or radiation
! calculate heat transfer via radiation
      IF(DES_RADI_EQ .AND. N_RAD .GT. 0) THEN
! Average the temperature
        Ts_RAD = Ts_RAD/N_RAD
        CALL DES_RADIATION(I, Ts_RAD, FOCUS)
      ENDIF
END SUBROUTINE CALC_THERMO_DES

```

D.7 Routine – DES_CONDUCTION

```

! Module name: DES_CONDUCTION
!
! Purpose:
!
! Author: J.Musser                               Date: 25-Jun-10
!
! Comments:
!
! REF: Batchelor and O'Brien, "Thermal or electrical conduction
!       through a granular material," Proceedings of the Royal Society
!       of London. Series A, Mathematical and Physical Sciences,
!       Vol. 355, no 1682, pp. 313-333, July 1977.
!
! REF: Rong and Horio, "DEM simulation of char combustion in a
!       fluidized bed," in Second International Conference on CFD in
!       the materials and Process Industries, Melbourne, 1999, pp.
!       65-70.
!
! REF: Xavier and Davidson, "Heat transfer to surfaces immersed in
!       fluidised beds, particularly tub arrays," in Fluidization:
!       Proceedings of the Second Engineering Foundation Conference,
!       Cambridge, England, 2-6 April, 1978, pp. 333-338.
!
! REF: Zhou, Yu, and Zulli, "Particle scale study of heat transfer in
!       packed and bubbling fluidized beds," AIChE Journal, Vol. 55,
!       no 4, pp 868-884, 2009.
!
! ~~~~~
! SUBROUTINE DES_CONDUCTION(I,J,C_DIST,FOCUS)
!
!       Use constant
!       Use des_thermo
!       Use discretelement
!       Use fldvar
!       Use funits
!       Use param1
!       Use physprop
!
!       IMPLICIT NONE
!
! Index value of particle I and it's neighbor J
!       INTEGER, INTENT(IN) :: I, J
! Distance between the particles centers
!       DOUBLE PRECISION, INTENT(IN) :: C_DIST
! Logical used for debugging
!       LOGICAL, INTENT(IN) :: FOCUS
!
! -----
! Local variables
! -----
! Index of fluid cell containing the center of particle I
!       INTEGER IJK
! Dummy integer indices for functions
!       INTEGER K, L
! Solid phase indices for the given particles
!       INTEGER I_M, J_M
!
! Distance between the particles surfaces

```

```

      DOUBLE PRECISION S_DIST
! Radius of smaller particle
      DOUBLE PRECISION MIN_RAD
! Radius of larger particle
      DOUBLE PRECISION MAX_RAD
! Rate of particle-particle conduction
      DOUBLE PRECISION Q_pp
! Rate of particle-fluid-particle conduction
      DOUBLE PRECISION Q_pfp
! Outer radius of region delineating particle-fluid-particle conduction
      DOUBLE PRECISION RD_OUT
! Inner radius of region delineating particle-fluid-particle conduction
      DOUBLE PRECISION RD_IN
! The radius of the fluid lens containing the larger particle
      DOUBLE PRECISION LENS_RAD
! Surface area of particle
      DOUBLE PRECISION A_S
! Thermo
      DOUBLE PRECISION Kg

! Identify the fluid cell containing particle I
      IJK = PIJK(I,4)

! Identify the solid phases of each particle
      I_M = PIJK(I,5)
      J_M = PIJK(J,5)

! Determine the radius of the larger and smaller particle
      MIN_RAD = MIN(DES_RADIUS(I), DES_RADIUS(J))
      MAX_RAD = MAX(DES_RADIUS(I), DES_RADIUS(J))

! Initialize the rates of conductive heat transfer
      Q_pp = ZERO
      Q_pfp = ZERO

! Calculate the particle-particle conduction
! REF: Batchelor and O'Brien, 1977 (MODIFIED)
      IF(DES_COND_EQ_PP .AND. C_DIST < (MAX_RAD + MIN_RAD) ) THEN
        Q_pp = 2.0d0 * K_eff(DES_K_s0(I_M),DES_K_s0(J_M)) * &
          (DES_T_s_NEW(J) - DES_T_s_NEW(I)) * &
          RADIUS(MAX_RAD, MIN_RAD)
! Assign the heat flux to both particles.
        Qpp(I) = Qpp(I) + Q_pp
        Qpp(J) = Qpp(J) - Q_pp
      ENDIF

! Calculate the particle-fluid-particle conduction
! REF: Rong and Horio, 1999 (MODIFIED)
      IF(DES_COND_EQ_PFP) THEN
! Calculate the radius of the fluid lens surrounding the larger particle
        LENS_RAD = MAX_RAD * (1.0D0 + FLPC)

! Calculate the outer radial distance (thickness) of the region for
! particle-fluid-particle heat conduction.
        RD_OUT = RADIUS( LENS_RAD, MIN_RAD)
! If the value returned is less than zero, then the fluid lens
! surrounding the larger particle does not intersect with the surface
! of the smaller particle. In this case, particle-fluid-particle
! conduction does not occur.
        IF( RD_OUT .GT. ZERO) THEN
! Calculate the distance from the line connecting the particles' centers
! to the point of contact between the two particles. This value is
! zero if the particles are not touching and is the radius of the

```

```

! shared contact area otherwise.
      RD_IN = ZERO
      IF(C_DIST < (MAX_RAD + MIN_RAD) ) &
        RD_IN = RADIUS(MAX_RAD, MIN_RAD)

! Thermal conductivity of gas phase
      IF(DES_CONTINUUM_COUPLED) THEN
        Kg = K_g(IJK)
      ELSE
        Kg = K_g0
      ENDIF

! Calculate the rate of heat transfer between the particles through the
! fluid using adaptive Simpson's rule to manage the integral.
      Q_pfp = Kg * (DES_T_s_NEW(J) - DES_T_s_NEW(I)) * &
        ADPT_SIMPSON(RD_IN, RD_OUT)
    ELSE
! Particles are not close enough to engage in particle-fluid-particle
! heat transfer.
      Q_pfp = ZERO
    ENDIF ! RD_OUT > ZERO
! Assign the heat flux to both particles.
      Qpfp(I) = Qpfp(I) + Q_pfp
      Qpfp(J) = Qpfp(J) - Q_pfp
    ENDIF

! Write debug messages
    IF(DEBUG_DES .AND. FOCUS) THEN
      WRITE(*, "(//5X,A)") 'From: DES_CONDUCTION -'
      WRITE(*, "(8X,A,D12.6)") 'Tp: ', DES_T_s_NEW(I)
      WRITE(*, "(8X,A,D12.6)") 'Qpp: ', Q_pp
      WRITE(*, "(8X,A,D12.6)") 'Qpfp: ', Q_pfp
      WRITE(*, "(5X,25('-'))")
    ENDIF

    RETURN

1000 FORMAT(/1X,70('*'),/' From: DES_COND_EQ',/, ' Message: ',&
  'Fatal Error calculating Qpfp! Check the log file for ',&
  'details!',/70('*'))

1001 FORMAT(1X,70('*'))

CONTAINS

!.....!
! Subroutine Procedure: FUNCTION RADIUS                                     !
!.....!
! Propose: Calculate the center line radius between two particles.      !
! Depending on what is given as input, this function calculates:        !
!   1) radius of contact area between two particles                    !
!   2) radius delineating particle-fluid-particle region.              !
!.....!
      DOUBLE PRECISION FUNCTION RADIUS(R1, R2)
! Radius values
      DOUBLE PRECISION, INTENT(IN) :: R1, R2
! Distance between particle centers
      DOUBLE PRECISION BETA
! Generic value
      DOUBLE PRECISION VALUE

! Calculate
      VALUE = (R1**2 - R2**2 + C_DIST**2)/(2.0d0 * R1 * C_DIST)
! Check to ensure that VALUE is less than or equal to one. If VALUE is

```

```

! greater than one, the triangle inequality has been violated. Therefore
! there is no intersection between the fluid lens surrounding the larger
! particle and the surface of the smaller particle.
! Thus, there is no particle-fluid-particle heat transfer.
      IF( VALUE .GT. 1.0d0) THEN
        RADIUS = -1.0d0
      ELSE
! Calculate beta (Law of cosines)
        BETA = ACOS( VALUE )
! Calculate the radius
        RADIUS = R1 * SIN(BETA)
      ENDIF

      RETURN
    END FUNCTION RADIUS

```

```

! .....!
! Subroutine Procedure: FUNCTION K_eff!
! .....!
! Propose: Calculate the effective thermal conductivity of two!
! particles with conductivities K1 and K2!
! .....!
      DOUBLE PRECISION FUNCTION K_eff(K1, K2)
! Thermal conductivities
      DOUBLE PRECISION, INTENT(IN) :: K1, K2

      K_eff = 2.0d0 * (K1*K2)/(K1 + K2)

      RETURN
    END FUNCTION K_eff

```

```

! .....!
! Function: F!
! .....!
! Purpose: This function defines the region of particle-fluid-particle!
! heat transfer. Note that this function develops a!
! singularity at the boundary of the contact region when two!
! particles are touching. This singularity is resolved by!
! making the assumption that the surfaces of two particles!
! never directly touch (c.f. Rong and Horio, 1999). By!
! default, it is assumed that the particles are separated by!
! a minimum length of  $4.0 \times 10^{-10}$  meters. This value may be!
! modified by specifying a different value in the mfix.dat!
! file under the variable name DES_MIN_COND_DIST.!
! .....!
! Note, the closer this value is to zero, the harder it will!
! be for the quadrature routine to converge.!
! .....!
      DOUBLE PRECISION FUNCTION F(R)
      DOUBLE PRECISION, INTENT(IN) :: R

      F = (2.0d0*Pi*R)/MAX((C_DIST - SQRT(MAX_RAD**2-R**2) - &
        SQRT(MIN_RAD**2-R**2)), DES_MIN_COND_DIST)

      IF( F.NE.F)PRINT*, 'F IS NAN'

      END FUNCTION F

```

```

! .....!
! Function: ADPT_SIMPSON!
! .....!
! Purpose: This function applies adaptive Simpson's Rule to solve the!
! definite integral of the function F.!
! .....!

```

```

!
!      *NOTE: This route will return the result of the method even !
!      if convergence has not been achieved. If this occurs, a    !
!      message will be written to the log file to notify the user. !
!.....!
      DOUBLE PRECISION FUNCTION ADPT_SIMPSON(A, B)

! Bounds of integration
      DOUBLE PRECISION, INTENT(IN) :: A, B
! Maximum recursive depth
      INTEGER, PARAMETER :: Kmax = 25
! Current depth of recursion
      INTEGER :: K
! Array storage for recursion
      DOUBLE PRECISION :: V(Kmax,6)
! Step size
      DOUBLE PRECISION :: H
! Simpson's Rule evaluated on the left and right intervals
      DOUBLE PRECISION :: lS, rS
! Value of the function F evaluate at the midpoints of the left and
! right intervals
      DOUBLE PRECISION :: rF, lF
! Local error bound
      DOUBLE PRECISION :: Err_BND
! Convergence bound
      DOUBLE PRECISION :: EPS = 10.0**(-2)

! Error indicating that an error has been specified to the user.
      LOGICAL, SAVE :: ADPT_SIMPSON_ERR = .FALSE.

! Initialize variables
      V(:, :) = 0.0d0 !
      ADPT_SIMPSON = 0.0d0 ! Integral value
      H = (B-A)/2.0d0 ! Dynamic interval length
! Calculate Simpson's Rule over the interval [A,B]
      lS = (F(A) + 4.0d0*F((A+B)/2.0d0) + F(B))*(H/3.0d0)
! Initialize the storage vector for the first pass
      V(1,:) = (/ A, H, F(A), F((A+B)/2.0d0), F(B), lS/)
      K = 1
! Enter recursion calculations
      DO
! Establish the new interval length
          H = V(K,2)/2.0d0
! Evaluate the function on the left interval
          lF = F(V(K,1) + H)
! Calculate Simpson's Rule over the left interval
          lS = (V(K,3) + 4.0d0*lF + V(K,4))*(H/3.0d0)
! Evaluate the function on the right interval
          rF = F(V(K,1) + 3.0d0*H)
! Calculate Simpson's Rule over the right interval
          rS = (V(K,4) + 4.0d0*rF + V(K,5))*(H/3.0d0)
! Evaluate the error bound
          Err_BND = (30.0d0*EPS*H)/(B-A)
! Check to see if conversion on the interval has been met
          IF( ABS(lS + rS - V(K,6)) .LT. Err_BND) THEN
! Update the integral value
              ADPT_SIMPSON = ADPT_SIMPSON + lS + rS + &
                  (1.0d0/15.0d0)*(lS + rS - V(K,6))
! Decrement the recursion counter
              K = K - 1
! If K=0, then integration has been successfully completed over the
! entire interval [A,B].
              IF( K == 0) RETURN

```

```

        ELSEIF( (K .GE. Kmax) .OR. &
            (H == (B-A)*(1.0d0/2.0d0)**(Kmax+3))) THEN
! Flag that the method did not converge.
        IF(.NOT.ADPT_SIMPSON_ERR)THEN
            WRITE(*,1000)
            WRITE(UNIT_LOG,1000)
            ADPT_SIMPSON_ERR = .TRUE.
        ENDIF
! Update the integral value
        ADPT_SIMPSON = ADPT_SIMPSON + lS + rS + &
            (1.0d0/15.0d0)*(lS + rS - V(K,6))
! Decrement the recursion counter
        K = K - 1
    ELSE
! Refine the subintervals through recursive splitting of the intervals
        V(K+1,:) = (/V(K,1) + 2.0d0*H, H, V(K,4), rF, V(K,5), rS/)
        V(K,:) = (/V(K,1), H, V(K,3), lF, V(K,4), lS/)
! Increment level counter
        K = K+1
    ENDIF
ENDDO

1000 FORMAT(/1X,70('*'),/' From: DES_COND_EQ',/, ' Message: ',      &
    'Integration of the particle-fluid-particle equation did ',      &
    'not',/' converge! No definite bound can be placed on the ',    &
    'error.',/' Future convergence messages will be suppressed!', &
    /1X,70('*'))

END FUNCTION ADPT_SIMPSON

END SUBROUTINE DES_CONDUCTION

```

```

! ~~~~~
! Module name: DES_CONVECTION
!
! Purpose: This routine is called from the discrete phase. It is used
! to determine the rate of heat transfer to the particle from the gas.
!
! Author: J.Musser                                Date: 16-Jun-10
!
! Comments:
!
! REF: Zhou, Yu, and Zulli, "Particle scale study of heat transfer in
!       packed and bubbling fluidized beds," AIChE Journal, Vol. 55,
!       no 4, pp 868-884, 2009.
!
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^
      SUBROUTINE DES_CONVECTION(I, INTERP_IJK, INTERP_WEIGHTS, FOCUS)

        Use constant
        Use des_thermo
        Use discretelement
        Use fldvar
        Use interpolation
        Use param1
        Use physprop

        IMPLICIT NONE

! Passed variables
!-----
! Index of particle being looped over
      INTEGER, INTENT(IN) :: I
! IJK indicies of fluid cells involved in interpolation
      INTEGER, INTENT(IN) :: INTERP_IJK(INTERP_ORDER**DIMN)
! Weights associated with interpolation
      DOUBLE PRECISION, INTENT(IN) :: INTERP_WEIGHTS(INTERP_ORDER**DIMN)
! Indicates that debugging information for the particle
      LOGICAL, INTENT(IN) :: FOCUS

! Local variables
!-----
! IJK value of cell containing particle I
      INTEGER IJK
! Convective heat transfer coefficient
      DOUBLE PRECISION GAMMA_CP
! Temperature of the gas
      DOUBLE PRECISION Tg
! Weight of specified IJK value
      DOUBLE PRECISION WEIGHT
! Loop counter
      INTEGER LC
! Surface area of particle
      DOUBLE PRECISION A_S

! Initialization
      IJK = PIJK(I,4)

! Obtain the temperature of the gas.
      IF(.NOT.DES_INTERP_ON)THEN
        Tg = T q(IJK)

```



```

ELSE
  Tg = ZERO
  DO LC=1, INTERP_ORDER**DIMN
    IJK = INTERP_IJK(LC)
    WEIGHT = INTERP_WEIGHTS(LC)
    Tg = Tg + (WEIGHT * T_g(IJK))
  ENDDO
ENDIF

! Obtain the convective heat transfer coefficient of the particle
CALL DES_CALC_GAMMA(I, GAMMA_CP)

! Calculate the surface area of the particle
A_S = 4.0d0 * Pi * DES_RADIUS(I)**2

! Calculate the rate of heat transfer to the particle
Qcv(I) = GAMMA_CP * A_S * (Tg - DES_T_s_NEW(I))

! Write out the debugging information.
IF(DEBUG_DES .AND. FOCUS) THEN
  WRITE(*,"(/5X,A)") 'From: DES_CONVECTION -'
  WRITE(*,"(8X,A,D12.6)") 'Tg: ',Tg
  WRITE(*,"(8X,A,D12.6)") 'Tp: ',DES_T_s_NEW(I)
  WRITE(*,"(8X,A,D12.6)") 'GAMMA_CP: ',GAMMA_CP
  WRITE(*,"(8X,A,D12.6)") 'Qcv: ',Qcv
  WRITE(*,"(5X,25(' ')/)")
ENDIF

RETURN

END SUBROUTINE DES_CONVECTION

```

```
! Subroutine: DES_Hgm
!  
!  
! Purpose: This routine is called from the continuum phase and  
! calculates the source term from the particles to the fluid. This  
! routine handles both the interpolated and non-interpolated options.  
!  
! Author: J.Musser Date: 15-Jan-11  
!  
! Comments:  
!  
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^  
SUBROUTINE DES_Hgm(S_C, S_P)  
  
USE compar  
Use constant  
Use des_thermo  
Use discretelement  
Use fldvar  
USE geometry  
USE indices  
Use interpolation  
Use paraml  
Use physprop  
  
IMPLICIT NONE  
  
! Source term on LHS. Must be positive.  
DOUBLE PRECISION, INTENT(INOUT) :: S_P(DIMENSION_3)  
! Source term on RHS  
DOUBLE PRECISION, INTENT(INOUT) :: S_C(DIMENSION_3)  
  
!-----  
! Local variables  
!-----  
  
! Index value of particle  
INTEGER NP  
! IJK value of cell containing particle NP  
INTEGER IJK  
! index to track accounted for particles  
INTEGER PC  
  
! Convective heat transfer coefficient  
DOUBLE PRECISION GAMMA_CP  
! Logical used for debugging  
LOGICAL FOCUS  
! Surface area of particle  
DOUBLE PRECISION A_S  
! IJK values of cells surrounding the particle, including boundary  
! conditions (i.e. periodic switches).  
INTEGER INTERP_IJK(INTERP_ORDER**DIMN)  
! Weight of corresponding IJK fluid cell [0,1]  
DOUBLE PRECISION INTERP_WEIGHTS(INTERP_ORDER**DIMN)  
  
! Weight of specifixed IJK value  
DOUBLE PRECISION WEIGHT  
! Loop counter  
INTEGER LC
```

```

! Initialize the particle counter
PC = 1
! Loop over the particles in the system
DO NP = 1, MAX_PIS
! Exit the loop if all the particles in the system have been looped over
IF(PC .GT. PIS) EXIT
! Cycle the loop if there is no particle associated with this index
IF(.NOT.PEA(NP,1)) CYCLE

! Set debug flag
FOCUS = .FALSE.
IF(NP.EQ.FOCUS_PARTICLE) FOCUS = .TRUE.

! Obtain the convective heat transfer coefficient of the particle
CALL DES_CALC_GAMMA(NP, GAMMA_CP)

! Calculate the surface area of the particle
A_S = 4.0d0 * Pi * DES_RADIUS(NP)**2

! Obtain the temperature of the gas.
IF(.NOT.DES_INTERP_ON)THEN

! Set the fluid cell index.
IJK = PIJK(NP,4)
! Calculate the source term components
S_P(IJK) = S_P(IJK) + ( GAMMA_CP * A_S )
S_C(IJK) = S_C(IJK) + ( GAMMA_CP * A_S * DES_T_s_NEW(NP) )

ELSE

! Determine the IJK values for the surrounding fluid cells and calculate
! the cell-centered interpolation weights.
CALL INTERPOLATE_CC(NP, INTERP_ORDER, &
INTERP_SCHEME, INTERP_IJK, INTERP_WEIGHTS, FOCUS)
! Distribute the thermal energy to/from the fluid cells
DO LC = 1, INTERP_ORDER**DIMN
! Set variable values
IJK = INTERP_IJK(LC)
WEIGHT = INTERP_WEIGHTS(LC)
! Portion the source term to cell IJK
S_P(IJK) = S_P(IJK) + WEIGHT * (GAMMA_CP * A_S)
S_C(IJK) = S_C(IJK) + WEIGHT * &
(GAMMA_CP * A_S * DES_T_s_NEW(NP))
ENDDO ! LC-loop
ENDIF ! End interpolation routine

! Reset the focus particle logical
FOCUS = .FALSE.
! Index the particle count by one
PC = PC + 1
ENDDO

END SUBROUTINE DES_Hgm

```

```

! ~~~~~
Subroutine: DES_CALC_GAMMA
!
! Purpose: Calculate the heat transfer coefficient (GAMMA_CP) for
particle-fluid heat transfer.
!
! Author: J.Musser                                Date: 16-Jun-10
!
! Comments:
!
! REF: Ranz, W.E. and Marshall, W.R., "Friction and transfer
coefficients for single particles and packed beds," Chemical
Engineering Science, Vol. 48, No. 5, pp 247-253, 1925.
! ~~~~~
SUBROUTINE DES_CALC_GAMMA(NP, GAMMA_CP)

USE compar
USE constant
USE des_thermo
USE discretelement
USE fldvar
USE geometry
USE indices
USE param1
USE physprop

IMPLICIT NONE

! Index value of particle
INTEGER, INTENT(IN) :: NP
! Convective heat transfer coefficient
DOUBLE PRECISION, INTENT(OUT) :: GAMMA_CP

!-----
! Local variables
!-----

! IJK value of cell containing particle NP
INTEGER IJK
! Fluid cell indices
DOUBLE PRECISION I, IMJK, IJMK, IJKM
! Double precision value for 1/3
DOUBLE PRECISION, PARAMETER :: THIRD = (1.0d0/3.0d0)
! Prandtl Number
DOUBLE PRECISION Pr
! Particle Reynolds Number
DOUBLE PRECISION Re_p
! Nusselt Number
DOUBLE PRECISION Nu_p
! Slip velocity between the particle and fluid
DOUBLE PRECISION SLIP_VEL(3)
! Magnitude of slip velocity
DOUBLE PRECISION SLIP_MAG
! Fluid velocity
DOUBLE PRECISION UGC, VGC, WGC

!-----
! Functions
!-----

DOUBLE PRECISION, EXTERNAL :: DES_DOTPRDCT

```

```

        INCLUDE 'fun_avg1.inc'
        INCLUDE 'function.inc'
        INCLUDE 'fun_avg2.inc'

! Initialization
        I = PIJK(NP,1)
        IJK = PIJK(NP,4)
        IMJK = IM_OF(IJK)
        IJMK = JM_OF(IJK)
        IJKM = KM_OF(IJK)

        SELECT CASE (TRIM(DES_CONV_CORR))

                CASE ('RANZ_1952') ! (Ranz and Mrshall, 1952)
! Initialize variables
                        SLIP_VEL(:) = ZERO
                        SLIP_MAG = ZERO
                        Re_p = ZERO
                        Nu_p = ZERO
! Gas velocity in fluid cell IJK
                        UGC = AVG_X_E(U_g(IMJK), U_g(IJK), 1)
                        VGC = AVG_Y_N(V_g(IJMK), V_g(IJK))
                        WGC = AVG_Z_T(W_g(IJKM), W_g(IJK))
! Calculate the slip velocity between the particle and fluid
                        SLIP_VEL(1) = UGC - DES_VEL_NEW(NP,1)
                        SLIP_VEL(2) = VGC - DES_VEL_NEW(NP,2)
                        IF(DIMN == 3) SLIP_VEL(3) = WGC - DES_VEL_NEW(NP,3)

! Calculate the magnitude of the slip velocity
                        SLIP_MAG = SQRT(DES_DOTPRDCT(SLIP_VEL,SLIP_VEL))

! Calculate the Prandtl Number
                        IF(K_G(IJK) > ZERO) THEN
                                PR = (C_PG(IJK)*MU_G(IJK))/K_G(IJK)
                                ELSE
                                PR = LARGE_NUMBER
                                ENDIF
! Calculate the particle Reynolds Number
                        IF(MU_G(IJK) > ZERO) THEN
                                Re_p = (2.0d0*DES_RADIUS(NP)*SLIP_MAG*RO_g(IJK)) / &
                                        MU_g(IJK)
                                ELSE
                                Re_p = LARGE_NUMBER
                                ENDIF

! Calculate the Nusselt Number
                        Nu_p = 2 + 0.6d0 * (Re_p)**HALF * (Pr)**THIRD

! Calculate the convective heat transfer coefficient
                        GAMMA_CP = (Nu_p * K_G(IJK))/(2.0d0 * DES_RADIUS(NP))

                CASE DEFAULT
                        WRITE(*,*) 'INVALID DES CONVECTION MODEL'
                        STOP
                        CALL MFIX_EXIT
        END SELECT

        RETURN

END SUBROUTINE DES_CALC_GAMMA

```

```

! ~~~~~!
! Module name: DES_RADIATION!
! Purpose:!
! Author: J.Musser Date: 25-Jun-10!
! Comment ENV:!
! REF: Batchelor and O'Brien, "Thermal or electrical conduction!
! through a granular material," Proceedings of the Royal Society!
! of London. Series A, Mathematical and Physical Sciences,!
! Vol. 355, no 1682, pp. 313-333, July 1977.!
! ~~~~~!
SUBROUTINE DES_RADIATION(I, T_ENV, FOCUS)

  Use constant
  Use des_thermo
  Use discretelement
  Use param1

  IMPLICIT NONE

! Index value of particle I
  INTEGER, INTENT(IN) :: I
! Average solids temperature in radiation domain
  DOUBLE PRECISION, INTENT(IN) :: T_ENV
! Logical used for debugging
  LOGICAL, INTENT(IN) :: FOCUS

!-----
! Local variables
!-----
! file name
  CHARACTER*64 :: FNAME
! logical used for testing is the data file already exists
  LOGICAL :: F_EXISTS
! Surface area of particle
  DOUBLE PRECISION A_S

! Calculate the surface area of the particle
  A_S = 4.0d0 * Pi * DES_RADIUS(I)**2

  Qrd(I) = SB_CONST * A_s * DES_EM(PIJK(I,5)) * &
    (T_ENV**4 - (DES_T_s_NEW(I))**4)

  IF(DEBUG_DES .AND. FOCUS)THEN
    WRITE(*, "(//5X,A)") 'From: DES_RADIATION -'
    WRITE(*, "(8X,A,D12.6)") 'Tp: ', DES_T_s_NEW(I)
    WRITE(*, "(8X,A,D12.6)") 'T_ENV: ', T_ENV
    WRITE(*, "(8X,A,D12.6)") 'Qrd: ', Qrd(I)
    WRITE(*, "(5X,25('-')/)")
  ENDIF

  RETURN

END SUBROUTINE DES_RADIATION

```

```
! Module name: DES_THERMO_NEWVALUES  
!  
! Purpose:  
!  
! Author: J.Musser Date: 16-Jun-10  
!  
! Comments:  
!  
^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^  
SUBROUTINE DES_THERMO_NEWVALUES(NP, FOCUS)  
  
    Use des_thermo  
    Use des_rxns  
    Use discretelement  
    Use param1  
    Use physprop  
  
    IMPLICIT NONE  
  
! Passed variables  
!-----  
! Index value of particle  
    INTEGER, INTENT(IN) :: NP  
! Logical indicating that the particle is of special interest  
    LOGICAL, INTENT(IN) :: FOCUS  
  
! Local variables  
!-----  
  
! index of solids phase  
    INTEGER M  
! Total amount of energy transfer TO the particle NP. If this value is  
! positive, then the particle is heating, if it is negative, then the  
! particle is cooling.  
    DOUBLE PRECISION Qtotal  
  
    DOUBLE PRECISION Qtotal_MAX  
    DOUBLE PRECISION Qpp_MAX, Qfpf_MAX, Qcv_MAX, Qrd_MAX, Quint_MAX  
  
! Logical for Adams-Bashfort integration.  
    LOGICAL,SAVE:: FIRST_PASS = .TRUE.  
    LOGICAL NOISY  
  
! Initialize local variables  
    Qcv_MAX = ZERO  
    Qpp_MAX = ZERO  
    Qfpf_MAX = ZERO  
    Qrd_MAX = ZERO  
    Quint_MAX = ZERO  
    Qtotal_MAX = ZERO  
  
! Initialize variables  
    Qtotal = ZERO  
    M = PIJK(NP,5)  
  
! Particle-fluid convection  
    IF(DES_CONV_EQ)THEN
```

```

!      WRITE(*,"(3X,A,F10.4)") 'Qcv:', Qcv(NP)
      Qtotal = Qtotal + Qcv(NP)
      Qcv_MAX = MAX( ABS(Qcv(NP)), Qcv_MAX)
      Qcv(NP) = ZERO
    ENDIF

! Particle-particle conduction
    IF(DES_COND_EQ_PP) THEN
!      WRITE(*,"(3X,A,F10.4)") 'Qpp:', Qpp(NP)
      Qtotal = Qtotal + Qpp(NP)
      Qpp_MAX = MAX( ABS(Qpp(NP)), Qpp_MAX)
      Qpp(NP) = ZERO
    ENDIF

! Particle-fluid-particle conduction
    IF(DES_COND_EQ_PFP) THEN
!      WRITE(*,"(3X,A,F10.4)") 'Qpfp:', Qpfp(NP)
      Qtotal = Qtotal + Qpfp(NP)
      Qpfp_MAX = MAX( ABS(Qpfp(NP)), Qpfp_MAX)
      Qpfp(NP) = ZERO
    ENDIF

! Energy from radiation
    IF(DES_RADI_EQ) THEN
!      WRITE(*,"(3X,A,F10.4)") 'Qrd:', Qrd(NP)
      Qtotal = Qtotal + Qrd(NP)
      Qrd_MAX = MAX( ABS(Qrd(NP)), Qrd_MAX)
      Qrd(NP) = ZERO
    ENDIF

! Energy from reaction
    IF(DES_SPECIES_EQ(M)) THEN
!      WRITE(*,"(3X,A,F10.4)") 'Qint', Qint(NP)
      Qtotal = Qtotal - Qint(NP)
      Qint_MAX = MAX( ABS(Qint(NP)), Qint_MAX)
      Qint(NP) = ZERO
    ENDIF

      Qtotal_MAX = MAX( ABS(Qtotal), Qtotal_MAX)

! Advance particle position, velocity
      IF (TRIM(DES_INTG_METHOD) .EQ. 'EULER') THEN
! First-order method
        DES_T_s_NEW(NP) = DES_T_s_OLD(NP) + &
          DTSOLID*(Qtotal / ( PMASS(NP) * DES_C_ps(NP) ))

        ELSEIF (TRIM(DES_INTG_METHOD) .EQ. 'ADAMS_BASHFORTH') THEN
! Second-order Adams-Bashforth scheme
          IF(FIRST_PASS == .TRUE.) THEN
            FIRST_PASS = .FALSE.
            DES_T_s_NEW(NP) = DES_T_s_OLD(NP) + &
              DTSOLID*(Qtotal / ( PMASS(NP) * DES_C_ps(NP) ))
            Qtotal_OLD(NP) = Qtotal / (PMASS(NP)*DES_C_ps(NP))
          ELSE
            DES_T_s_NEW(NP) = DES_T_s_OLD(NP) + &
              ( 1.5d0 * (Qtotal/(PMASS(NP)*DES_C_ps(NP))) - &
                0.5d0 * Qtotal_OLD(NP) ) * DTSOLID
            Qtotal_OLD(NP) = Qtotal / (PMASS(NP)*DES_C_ps(NP))
          ENDIF
        ENDIF

! Update the old temperature value
      DES_T_s_OLD(NP) = DES_T_s_NEW(NP)

      RETURN
    END SUBROUTINE DES_THERMO_NEWVALUES

```



```

! ~~~~~!
! Module name: THERMO_NBR!
! Purpose: Check the data provided for the des!
! Author: J.Musser! Date: 17-Feb-11!
! Comments:~::~:
! ~~~~~!
SUBROUTINE THERMO_NBR(L,LL,DIST)

  Use des_thermo
  Use discretelement

  IMPLICIT NONE

  INTEGER, INTENT(IN) :: L, LL

  DOUBLE PRECISION, INTENT(IN) :: DIST

  INTEGER NEIGH_L, NEIGH_LL

  IF(DIST .LE. NBRHD_SZ) THEN

    THERMO_NBRHD(L,1) = THERMO_NBRHD(L,1) + 1
    THERMO_NBRHD(LL,1) = THERMO_NBRHD(LL,1) + 1

    NEIGH_L = THERMO_NBRHD(L,1)
    NEIGH_LL = THERMO_NBRHD(LL,1)

    IF(NEIGH_L .LE. MN) THEN
      THERMO_NBRHD(L,NEIGH_L+1) = LL
    ELSE
      WRITE(*,1002)L,MN
    ENDIF

    IF(NEIGH_LL .LE. MN) THEN
      THERMO_NBRHD(LL,NEIGH_LL+1) = L
    ELSE
      WRITE(*,1002)LL,MN
    ENDIF

  ENDIF

  RETURN

1002 FORMAT(/1X,70('*')/,1X,'From: THERMO_NBR -',/ &
  ' Message: The number of particles in the thermodynamic', &
  ' neighborhood',/ ' of particle ',I6,' has exceeded',I3,&
  /1X,70('*'))

END SUBROUTINE THERMO_NBR

```

```

! ~~~~~
! Subroutine: SET_INTERPOLATION_STENCIL_CC
!
! Purpose:
!
! Author: J.Musser                               Date:
!
! Comments:
! ~~~~~
SUBROUTINE SET_INTERPOLATION_STENCIL_CC(NP, PC, SCHEME, ORDER, &
    IW, JS, KB, FOCUS)

    USE discretelement
    USE geometry
    USE param1

    IMPLICIT NONE

! I, J, K indices of the cell containing the particle.
    INTEGER, INTENT(IN) :: PC(3)
! particle number
    INTEGER, INTENT(IN) :: NP
! interpolation order
    INTEGER, INTENT(IN) :: ORDER
! interpolation scheme
    CHARACTER*5, INTENT(IN) :: SCHEME
! These values indicate the I,J,K starting indices used to select the
! nodes for interpolation.
    INTEGER, INTENT(OUT) :: IW, JS, KB
! flag to tell whether local debugging was called in drag_fgs
    LOGICAL, INTENT(IN) :: FOCUS

!-----
! Local variables
!-----
! indices
    INTEGER I, J, K, II, JJ, KK
    INTEGER I_SHIFT, J_SHIFT, K_SHIFT, IE, JN, KTP
! Identifies the number of nodes to the left and right of the particle
! to be used in the interpolation. These values are calculated based
! on the order of the interpolation scheme selected.
    INTEGER OB2L, OB2R

!-----
    OB2L = (ORDER+1)/2
    OB2R = ORDER/2
! Determine the shift index necessary to account for the quadrant of
! the fluid cell where the particle is located.
    IF( DES_POS_NEW(NP,1) <= XE(PC(1))-HALF*DX(PC(1))) THEN
        I_SHIFT = 0
    ELSE
        I_SHIFT = 1
    ENDIF
    IF( DES_POS_NEW(NP,2) <= YN(PC(2))-HALF*DY(PC(2))) THEN
        J_SHIFT = 0
    ELSE
        J_SHIFT = 1
    ENDIF

```

```

      IF(DIMN == 2) THEN
        K_SHIFT = 0
      ELSE
        IF( DES_POS_NEW(NP,3) <= ZT(PC(3))-HALF*DZ(PC(3))) THEN
          K_SHIFT = 0
        ELSE
          K_SHIFT = 1
        ENDIF
      ENDIF

! Calculate the west and east I indices to be used.
!-----
! Restrict the west I index to a minimum of 1
  IW = MAX( 1, (PC(1) - OB2L + I_SHIFT))
! Restrict the east I index to a maximum of IMAX1
  IE = MIN( IMAX2, PC(1) + (OB2R-1) + I_SHIFT)
  IF(.NOT.DES_PERIODIC_WALLS_X) THEN
! If the YZ walls are not periodic, ensure that the indices used for
! interpolation stay within the domain. This may require a shift in the
! indices for cells near the walls and interpolation schemes of high
! order.
    IF (IE .EQ. IMAX2) IW = IMAX2 - ORDER + 1
  ELSE
! If the YZ walls are periodic, the starting index can be less than 1.
! This is accounted for when filling GSTENCIL. corrected later.
    IF (IW .EQ. 1) IW = IE - ORDER + 1
  ENDIF

! Calculate the south and north J indices to be used.
!-----
! Restrict the south J index to a minimum of 1
  JS = MAX( 1, PC(2) - OB2L + J_SHIFT)
! Restrict the north J index to a maximum of JMAX1
  JN = MIN( JMAX2, PC(2) + (OB2R-1) + J_SHIFT)
  IF(.NOT.DES_PERIODIC_WALLS_Y) THEN
! Shift indices for non periodic boundaries if needed.
    IF (JN .EQ. JMAX2) JS = JMAX2 - ORDER + 1
  ELSE
! Shift indices for periodic boundaries if needed.
    IF (JS .EQ. 1 ) JS = JN - ORDER + 1
  ENDIF

! Calculate the bottom and top K indices to be used.
!-----
  IF(DIMN == 2) THEN
! If 2 dimension simulation, set the bottom index to 1.
    KB = 1
  ELSE
! Restrict the bottom K index to a minimum of 1
    KB = MAX( 1, PC(3) - OB2L + K_SHIFT)
! Restrict the top K index to a maximum of KMAX1
    KTP = MIN( KMAX2, PC(3) + (OB2R-1) + K_SHIFT)
    IF(.NOT.DES_PERIODIC_WALLS_Z) THEN
! Shift indices for non periodic boundaries if needed.
      IF (KTP .EQ. KMAX1) KB = KTP - ORDER + 1
    ELSE
! Shift indices for periodic boundaries if needed.
      IF (KB .EQ. 1 ) KB = KTP - ORDER + 1
    ENDIF
  ENDIF

  RETURN
END SUBROUTINE SET_INTERPOLATION_STENCIL_CC

```

```
! SUBROUTINE: INTERPOLATE_CC !  
!  
! Purpose: !  
!  
! Author: J.Musser Date: 13-Jan-11 !  
!  
! Comments: !  
!  
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^ !  
      SUBROUTINE INTERPOLATE_CC(NP, ORDER, SCHEME, INTP_IJK, &  
                                INTP_WEIGHTS, FOCUS)  
  
      USE compar  
      USE discretelement  
      USE geometry  
      USE indices  
      USE param  
      USE paraml  
  
      IMPLICIT NONE  
  
! Particle index number  
      INTEGER, INTENT(IN) :: NP  
! Interpolation order  
      INTEGER, INTENT(IN) :: ORDER  
! Interpolation scheme  
      CHARACTER*5, INTENT(IN) :: SCHEME  
! Local debugging flag  
      LOGICAL, INTENT(IN) :: FOCUS  
  
! IJK values of cells. These have already been adjusted for periodic  
! and non-periodic boundary conditions.  
      INTEGER, INTENT(OUT) :: INTP_IJK(ORDER**DIMN)  
! Weights associated with the IJK cells in INTP_IJK  
      DOUBLE PRECISION, INTENT(OUT) :: INTP_WEIGHTS(ORDER**DIMN)  
  
!-----  
! Local variables  
!-----  
  
! Starting grid indices used in interpolation  
      INTEGER IW, JS, KB  
  
! Weights associated with the nodes used for interpolation. These values  
! only need to be returned with interpolating routine is invoked from  
! the continuum phase.  
      DOUBLE PRECISION, POINTER :: WEIGHTS_CC (:,:, :)  
  
! indices  
      INTEGER I, J, K, II, JJ, KK, IJK  
  
! Loop counter  
      INTEGER LC  
  
! geometry and field stencils for cell-center interpolations  
      DOUBLE PRECISION STNCL_GEMTY (ORDER, ORDER, MAX(1, ORDER*(DIMN-2)), DIMN)  
      DOUBLE PRECISION STNCL_FEILD (ORDER, ORDER, MAX(1, ORDER*(DIMN-2)))  
  
      DOUBLE PRECISION INTERP scalar
```

```

!-----

      INCLUDE 'function.inc'

! Obtain the starting cell index values for interpolation around
! particle NP
      CALL SET_INTERPOLATION_STENCIL_CC(NP, PIJK(NP,1:3), SCHEME, &
          ORDER, IW, JS, KB, FOCUS)

      LC = 0
      DO K = 1, (3-DIMN)*1+(DIMN-2)*ORDER
          DO J = 1, ORDER
              DO I = 1, ORDER

! increment the loop counter
                  LC = LC + 1

! Shift loop indicies to the correct values
                  II = IW + I-1
                  JJ = JS + J-1
                  KK = KB + K-1

! Adjust for boundary conditions.
                  IF (DES_PERIODIC_WALLS_X) THEN
                      IF (II .LT. IMIN1) THEN
! Shift from the east side of the domain to the west side.
                          II = IMAX2 + (II-IMIN1)
                          STNCL_GEMTY(I,J,K,1) = XE(II) - HALF*DX(II) - XLENGTH
                      ELSEIF (II .GT. IMAX1) THEN
! Shift for the west side of the domain to the east side.
                          II = II - IMAX
                          STNCL_GEMTY(I,J,K,1) = XLENGTH + XE(II) - HALF*DX(II)
                      ELSE
! No shift needed. Use actual node location.
                          STNCL_GEMTY(I,J,K,1) = XE(II) - HALF*DX(II)
                      ENDIF
                  ELSE
! If the YZ plane is not periodic, calculate the position of the node.
                          STNCL_GEMTY(I,J,K,1) = XE(II) - HALF*DX(II)
! Due to the restrictions on non periodic 1 <= II and II <= IMAX2.
! Shift the II east/west to reflect the cell value at the boundary.
                          IF (II .EQ. 1) THEN
                              II = IMIN1
                          ELSEIF (II .EQ. IMAX2) THEN
                              II = IMAX1
                          ENDIF
                      ENDIF
                  IF (DES_PERIODIC_WALLS_Y) THEN
                      IF (JJ .LT. JMIN1) THEN
! Shift from the north side of the domain to the south side.
                          JJ = JMAX2 + (JJ-JMIN1)
                          STNCL_GEMTY(I,J,K,2) = YN(JJ) - HALF*DY(JJ) - YLENGTH
                      ELSEIF (JJ .GT. JMAX1) THEN
! Shift from the south side of the domain to the north side.
                          JJ = JJ - JMAX
                          STNCL_GEMTY(I,J,K,2) = YLENGTH + YN(JJ) - HALF*DY(JJ)
                      ELSE
! No shift needed. Use the nodes actual position.
                          STNCL_GEMTY(I,J,K,2) = YN(JJ) - HALF*DY(JJ)
                      ENDIF
                  ELSE
! If the XZ plane is not periodic, calculate the position of the node.
                          STNCL_GEMTY(I,J,K,2) = YN(JJ) - HALF*DY(JJ)

```

```

! Due to the restrictions on non periodic 1 <= II and II <= IMAX2.
! Shift the II east/west to reflect the cell value at the boundary.
      IF(JJ .EQ. 1) THEN
        JJ = JMIN1
      ELSEIF(JJ .EQ. JMAX2) THEN
        JJ = JMAX1
      ENDIF
    ENDIF
    IF (DIMN .EQ. 3) THEN
      IF (DES_PERIODIC_WALLS_Z) THEN
        IF(KK .LT. KMIN1) THEN
! Shift from the top side of the domain to the bottom side.
          KK = KMAX1 + (KK-KMIN1)
          STNCL_GEMTY(I,J,K,3) = ZT(KK) - HALF*DZ(KK) - ZLENGTH
        ELSEIF(KK .GT. KMAX1) THEN
! Shift from the bottom side of the domain to the top side.
          KK = KK - KMAX
          STNCL_GEMTY(I,J,K,3) = ZLENGTH + ZT(KK) - HALF*DZ(KK)
        ELSE
! No shift needed. Use actual node location.
          STNCL_GEMTY(I,J,K,3) = ZT(KK) - HALF*DZ(KK)
        ENDIF
      ELSE
! If the XY plane is not periodic, calculate the position of the node.
          STNCL_GEMTY(I,J,K,3) = ZT(KK) - HALF*DZ(KK)
! Due to the restrictions on non periodic 1 <= II and II <= IMAX2.
! Shift the II east/west to reflect the cell value at the boundary.
          IF(KK .EQ. 1) THEN
            KK = KMIN1
          ELSEIF(KK .EQ. KMAX2) THEN
            KK = KMAX1
          ENDIF
        ENDIF
      ELSE
        KK = 1
      ENDIF
! Store the IJK in the interp array
      INTP_IJK(LC) = FUNIJK(II,JJ,KK)
! Assign a dummy value for the feild variable
      STNCL_FEILD(I,J,K) = 1.0d0
    ENDDO
  ENDDO
ENDDO

! Call the interpolation routine. If the call to this routine originates
! from the continuum phase, the interpolation weights are of interest.
! Otherwise, the interpolated scalar value (INTERP_scalar) is desired.
  IF(DIMN.EQ.2) THEN
    CALL interpolator( STNCL_GEMTY(1:ORDER, 1:ORDER, 1, 1:DIMN), &
      STNCL_FEILD(1:ORDER, 1:ORDER, 1), &
      DES_POS_NEW(NP,1:2), INTERP_scalar, ORDER, SCHEME, WEIGHTS_CC )
  ELSE
    CALL interpolator( STNCL_GEMTY(1:ORDER, 1:ORDER, 1:ORDER, 1:DIMN), &
      STNCL_FEILD(1:ORDER, 1:ORDER, 1:ORDER), &
      DES_POS_NEW(NP,:), INTERP_scalar, ORDER, SCHEME, WEIGHTS_CC )
  ENDIF

! Store interpolation weights in an array for calling routine
  LC = 0
  DO K = 1, (3-DIMN)*1+(DIMN-2)*ORDER
    DO J = 1, ORDER
      DO I = 1, ORDER
! increment the loop counter

```

```

        LC = LC + 1
        INTP_WEIGHTS(LC) = WEIGHTS_CC(I,J,K)
    ENDDO
ENDDO
ENDDO

! Local debugging
IF(FOCUS .AND. DEBUG_DES)THEN
    WRITE(*,"(3X,A,1X,A3,4X,A,I2)") &
        'Interpolation Scheme:',SCHEME,'Interpolation Order:',ORDER
    WRITE(*,"(3X,A,I5,3X,A,I6)")'Particle: ',NP,'IJK: ',PIJK(NP,4)
    WRITE(*,"(/5X,'|',29('-'),'|')")
    WRITE(*,"(5X,A)")'| Fluid Cell | Interp. Weight |'
    WRITE(*,"(5X,'|',12('-'),'|',16('-'),'|')")
    DO LC = 1, ORDER**DIMN
        WRITE(*,"(5X,'|',2X,I8,2X,'|',2X,F12.10,2X,'|')")&
            INTP_IJK(LC), INTP_WEIGHTS(LC)
    ENDDO
    WRITE(*,"(5X,'|',29('-'),'|'//)")
ENDIF ! Local Debugging

END SUBROUTINE INTERPOLATE_CC

```



```

! 1) [SHRINKING_CORE] : The outer radius of the particle remains
!     constant while an unreacted core shrinks during the reaction.
!     In this model, a secondary radius (CORE_RAD) is tracked for
!     each particle to represent the radius of the core.
! 2) SHRINKING_PARTICLE : As components of the particle are consumed,
!     the size of the particle reduces to maintain a constant
!     density.
! 3) PROGRESSIVE_CONVERSION : The size of the particle remains constant
!     but the density of the particle is changed to reflect the
!     consumption of the components of the particle.
CHARACTER*64 REACTION_MODEL

! If using the shrinking core model, this term represents the radius
! of the unreacted core.
DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: CORE_RAD
! Constant density of the core for the shrinking core model. The
! Ro_Sol variable is adjusted to reflect a 'bulk density' of the
! particle.
DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: CORE_Rho

! Previous time step's rate of change. Used for Adams-Bashforth
! time integration scheme.
! 1) particle mass
DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: dMdt_OLD
! 2) particle species mass
DOUBLE PRECISION, DIMENSION(:,:), ALLOCATABLE :: dXdT_OLD
! 3) radius of unreacted core
DOUBLE PRECISION, DIMENSION(:), ALLOCATABLE :: dRdt_OLD

END MODULE DES_RXNS

```

```
! ~~~~~  
!  
! Module name: CHECK_DES_RXNS  
!  
! Purpose:  
!  
!  
! Author: J.Musser Date: 17-Jun-11  
!  
! Comments:  
!  
! ~~~~~  
  
SUBROUTINE CHECK_DES_RXNS  
  
    Use compar  
    USE des_rxns  
    Use discretelement  
    Use funits  
  
    Use run  
  
    IMPLICIT NONE  
  
!-----  
! Local variables  
!-----  
! Dummy loop indices for solids phase and species  
    INTEGER M, N  
  
! Logical indicating that an error message has been sent to the user.  
    LOGICAL WARNED  
  
    FIRST_CALL = .TRUE.  
  
    WRITE(*,'(lX,A)') '----- START CHECK_DES_RXNS ----->'  
  
! Initialize MAX DES_NMAX. This is the maximum number of species found  
! over all solids phases. This is used for allocating DES_X_s  
    MAX_DES_NMAX = 1  
  
! Check DES_NMAX - this value must be defined if DES_SPECIES_EQ(M) is  
! true.  
    DO M = 1, DES_MMAX  
        IF (DES_NMAX(M) == UNDEFINED_I) THEN  
            ! If the species equation is being solved, then the user must specify  
            ! the number of species in the discrete solids phase.  
                IF (DES_SPECIES_EQ(M)) THEN  
                    WRITE(*,1000)M  
                    IF(DMP_LOG) WRITE(UNIT_LOG,1000)M  
                    CALL MFIX_EXIT(myPE)  
                ELSE  
                    ! Set the species count to be 1 if the speices count is not being  
                    ! solved.  
                        DES_NMAX(M) = 1  
                    ENDIF  
                ELSE  
                    MAX_DES_NMAX = MAX(MAX_DES_NMAX, DES_NMAX(M))  
                    ! Ensure that the number of species specified by the user is below the  
                    ! max limit.  
                        IF (DES_NMAX(M) > DIM_N_S) THEN
```

```

        WRITE(*,1001)M
        IF(DMP_LOG) WRITE(UNIT_LOG,1001)M
        CALL MFIX_EXIT(myPE)
    ENDIF
ENDIF

ENDDO

! Initialize error message flag.
WARNED = .FALSE.
! Check if the molecular weights are provided by the user.
DO M = 1, DES_MMAX
    IF (DES_SPECIES_EQ(M)) THEN
        DO N = 1, DES_NMAX(M)
            IF (DES_MW_S(M,N) == UNDEFINED) THEN

! If the molecular weight has not been provided in the mfix.dat file,
! notify the user that it will be obtained from the thermodynamic
! database.

                IF(.NOT.WARNED)THEN
                    WRITE(*,1005)
                    IF(DMP_LOG) WRITE(UNIT_LOG, 1005)
                    WARNED = .TRUE.
                ENDIF
                WRITE(*, 1006) M, N
                IF(DMP_LOG) WRITE(UNIT_LOG) M, N
            ENDIF
        ENDDO
    ENDIF
    IF(WARNED)THEN
        WRITE(*,1007)
        IF(DMP_LOG) WRITE(UNIT_LOG,1007)
    ENDIF
ENDIF

! If the molecular weight is specified for species with an index greater
! than DES_NMAX, flag the error and exit.
DO N = DES_NMAX(M) + 1, DIM_N_S
    IF (DES_MW_S(M,N) /= UNDEFINED) THEN
        WRITE(*,1008) M
        IF(DMP_LOG) WRITE(UNIT_LOG,1008) M
    ENDIF
ENDDO
ENDIF
ENDDO

! Set the flag identifying that at least one of the species equations
! are being solved.
ANY_DES_SPECIES_EQ = ANY(DES_SPECIES_EQ(:DES_MMAX))

WRITE(*,'(1X,A)') '<----- END CHECK_DES_RXNS -----'

RETURN

! Error Messages
!-----
1000 FORMAT(/1X,70('*')/, ' From: CHECK_DES_RXNS',/, ' Message: ', &
'Number of species for discrete phase ',I2,', not specified.', &
/1X,70('*')/)

1001 FORMAT(/1X,70('*')/, ' From: CHECK_DES_RXNS',/, ' Message: ', &
'DES_NMAX is too large for discrete phase ',I2,',',/1X,70('*'))

1002 FORMAT(/1X,70('*')/, ' From: CHECK_DES_RXNS',/, ' Message:', &
' Species molecular weight is undefinded for phase ',I2,',',/ &

```

```

        ' species ',I3,' in mfix.dat file. These values will be',      &
        ' obtained from the',/'thermodynamic database.',/1X,70('*')/)

1005 FORMAT(/1X,70('*')/, ' From: CHECK_DES_RXNS',/, ' Message:',      &
        ' Molecular weight not defined for the following:')

1006 FORMAT(4X,'Solids phase: ',I2,' Species: ',I3)

1007 FORMAT(' The thermodynamic databases will be consulted.',/      &
        1X,70('*')/)

1008 FORMAT(/1X,70('*')/, ' From: CHECK_DES_RXNS',/, ' Message:',      &
        ' DES_MW_s is defined for an index value greater than',      &
        ' DES_NMAX for',/' solids phase ',I2,'. Check mfixdat file.',/&
        1X,70('*')/)

END SUBROUTINE CHECK_DES_RXNS

```

```

! VVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVVV !
! Function: DES_CALC_H                                              !
!                                                                    !
! Purpose: Calculate the enthalpy for des_rrates subroutine.      !
!                                                                    !
! Author: J.Musser                                                  Date: 16-Jun-10    !
!                                                                    !
! Comments:                                                         !
!                                                                    !
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^ !
DOUBLE PRECISION FUNCTION DES_CALC_H(NP, N)

USE constant
USE des_rxns
USE des_thermo
USE discretelement

IMPLICIT NONE

! Particle index
INTEGER, INTENT(IN) :: NP
! Species index
INTEGER, INTENT(IN) :: N
! Index for the discrete solids phase of the particle
INTEGER M
! Reference temperature
DOUBLE PRECISION ICpoR
DOUBLE PRECISION, EXTERNAL :: CALC_ICpoR

M = PIJK(NP,5)

! Enthalpy
ICpoR = CALC_ICpoR(DES_T_s_NEW(NP), DES_Thigh_s(M,N), &
    DES_Tlow_s(M,N), DES_Tcom_s(M,N), DES_Ahigh_s(1,M,N), &
    DES_Alow_s(1,M,N))

DES_CALC_H = (DES_Hrefor_s(M,N)+(ICpoR-DES_IC_PsrefoR(M,N))) * &
    GAS_CONST_cal / DES_MW_s(M,N)

END FUNCTION DES_CALC_H

```

```
! ~~~~~  
! Subroutine name: PHYSICAL_PROP  
!  
! Purpose: Calculate physical properties that vary with time.  
!  
! Author: J.Musser                               Date: 09-May-11  
!  
! ^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^^~  
      SUBROUTINE DES_PHYSICAL_PROP(NP, FOCUS)  
  
        Use des_rxns  
        Use des_thermo  
        Use discretelement  
        Use funits  
        Use param  
        Use paraml  
        Use physprop  
        Use run  
  
        IMPLICIT NONE  
  
! Passed Variables  
!-----  
! Index of particle  
    INTEGER, INTENT(IN) :: NP  
! Logical indicating to write additional data about the particle for  
! debugging purposes.  
    LOGICAL, INTENT(IN) :: FOCUS  
  
! Local Variables  
!-----  
! Gas constant  
    DOUBLE PRECISION, PARAMETER :: RGAS = 1.987207D0 !cal/mol.K  
! Dummy indices  
    INTEGER M, N  
! error indicator  
    INTEGER IER  
  
! External fuctions  
!-----  
! Calculate the specific heat from polynomial data obtained from the  
! thermodynamic databases.  
    DOUBLE PRECISION , EXTERNAL :: calc_CpoR  
  
! Get the solids phase of the particle  
    M = PIJK(NP,5)  
  
! Specific heat  
!-----  
! This only needs calculated when solving the energy equations.  
    IF(DES_ENERGY_EQ) THEN  
! If a constant value specific heat has not been defined in the mfix.dat  
! file, calculate the temperature dependent value based on data from the  
! thermodynamic databases.  
        IF (DES_C_PS0(M) == UNDEFINED) THEN  
! Read the thermodynamic database if it has not already been done.  
            IF(.NOT.DATABASE_READ) CALL READ_DATABASE(IER)  
            DES_C_PS(NP) = ZERO  
! Calculate the specific heat based on the species composition of the  
! particle and the data from the thermodynamic databases.
```

```

      DO N = 1, DES_NMAX(M)
        DES_C_PS(NP) = DES_C_PS(NP) + DES_X_s(NP,N) *      &
          calc_CpoR(DES_T_s_NEW(NP), DES_Thigh_s(M, N),    &
            DES_Tlow_s(M, N), DES_Tcom_s(M, N),
&
            DES_Ahigh_s(1,M,N), DES_Alow_s(1,M,N)) *      &
            RGAS/DES_MW_s(M,N)
      ENDDO
! Convert to SI units if needed.
      IF (UNITS == 'SI') DES_C_PS(NP) = 4183.925D0*DES_C_PS(NP)
      ELSE
! If a constant value specific heat has been assigned to the particle
! in the mfix.dat file, use this value.
        DES_C_PS(NP) = DES_C_PS0(M)
      ENDIF
    ENDIF

!      WRITE(*,"(3X,A,I2,A,F10.6)") 'DES_C_PS(',NP,'): ',DES_C_PS(NP)

    RETURN

  END SUBROUTINE DES_PHYSICAL_PROP

```

[illegible]


```

      DOUBLE PRECISION Tg
! Rate of gas phase species production (g/s)
      DOUBLE PRECISION DES_R_gp(NMAX(0))
! Rate of gas phase species consumption per species concentration (g/s)
      DOUBLE PRECISION DES_RoX_gc(NMAX(0))
! Rate of enthalpy transfer
      DOUBLE PRECISION RxH_xfr
! Heat of reaction
      DOUBLE PRECISION HOR
! Mass generated
      DOUBLE PRECISION MASS_GEN

      DOUBLE PRECISION R_tmp(0:DES_MMAX, 0:DES_MMAX)
      DOUBLE PRECISION X_tmp(0:DES_MMAX, 0:DES_MMAX, Dimension_n_all)

      DOUBLE PRECISION, EXTERNAL :: calc_h
      DOUBLE PRECISION, EXTERNAL :: DES_CALC_H

!.....!
! Reaction specific variables:
!.....!

! Function subroutines
!-----
      LOGICAL COMPARE

      INCLUDE 'fun_avg1.inc'
      INCLUDE 'function.inc'
      INCLUDE 'fun_avg2.inc'
      INCLUDE 'usrnlst.inc'

! Set the mass phase of the particle
      PARTICLE_PHASE = PIJK(NP,5)

! Return if the species equations for the particle's phase are not
! being solved.
      IF(.NOT.DES_SPECIES_EQ(PARTICLE_PHASE)) RETURN

! Initialize variables
      R_tmp = UNDEFINED
! Set the fluid cell of the particle
      IJK = PIJK(NP,4)
! Set the particle temperature
      Tp = DES_T_s_NEW(NP)

      DES_R_gp(:) = ZERO
      DES_RoX_gc(:) = ZERO
      DES_R_sp(NP,:) = ZERO
      DES_R_sc(NP,:) = ZERO

! User input is required in sections A,1,2,3.

!AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA!
!
! A. Set gas phase quantities.
!
! The gas phase species information is set to the array Xg(:) and
! the gas phase temperature is set to the variable Tg.
!
! Additional quantites may also be set by using the function
!
```



```

! <----- No user input is required below this line -----> !
!=====!

      IF(CALLER == 'GAS') THEN
! Store the transfer quantities in the continuum variables
!-----
      DO N=1,NMAX(0)
        CALL TO_FIELD(R_gp(:,N), DES_R_gp(N))
        CALL TO_FIELD(RoX_gc(:,N), DES_RoX_gc(N))
      ENDDO

! Calculate the rate of mass generate in g/(s.cm^3) for the gas phase.
!-----
      IF (SPECIES_EQ(0)) THEN
! If the species equations are being solved for the gas phase, then
! the total rate of mass generate is the sum of the production and
! consumption terms for each species.
      DO N=1,NMAX(0)
        MASS_GEN = DES_R_gp(N) - DES_RoX_gc(N)*Xg(N)
      ENDDO
      ELSE
! If the species equations are not being solved, use the values provided
! in the R_tmp array.
      IF(R_tmp(0,PARTICLE_PHASE) .NE. UNDEFINED) THEN
        MASS_GEN = R_tmp(0,PARTICLE_PHASE)
      ELSEIF(R_tmp(PARTICLE_PHASE,0) .NE. UNDEFINED) THEN
        MASS_GEN = R_tmp(PARTICLE_PHASE,0)
      ENDIF
      ENDIF
      CALL TO_FIELD(SUM_R_G, MASS_GEN)
    ENDIF

! Calculate the rate enthalpy of transfer from material exchange
!-----
      RxH_xfr = ZERO
! Mass transfer is occurring.
      IF(R_tmp(0,PARTICLE_PHASE) .NE. UNDEFINED) THEN
! solids phase species >> gas phase species
      IF(R_tmp(0, PARTICLE_PHASE) > ZERO) THEN
        DO N = 1, NMAX(0)
          RxH_xfr = RxH_xfr + R_tmp(0,PARTICLE_PHASE) * &
            X_tmp(0,PARTICLE_PHASE,N) * CALC_H(IJK,0,N)
        ENDDO
! gas phase species >> solids phase species
      ELSE
        DO N = 1, DES_NMAX(PARTICLE_PHASE)
          RxH_xfr = RxH_xfr + R_tmp(0,PARTICLE_PHASE) * &
            X_tmp(0,PARTICLE_PHASE,N) * DES_CALC_H(NP,N)
        ENDDO
      ENDIF
      ELSEIF(R_tmp(PARTICLE_PHASE,0) .NE. UNDEFINED) THEN
! gas phase species >> solids phase species
      IF(R_tmp(PARTICLE_PHASE,0) > ZERO) THEN
        DO N = 1, DES_NMAX(PARTICLE_PHASE)
          RxH_xfr = RxH_xfr - R_tmp(PARTICLE_PHASE,0) * &
            X_tmp(PARTICLE_PHASE,0,N) * DES_CALC_H(NP,N)
        ENDDO
! solids phase species >> gas phase species
      ELSE
        DO N = 1, NMAX(0)
          RxH_xfr = RxH_xfr - R_tmp(PARTICLE_PHASE,0) * &
            X_tmp(PARTICLE_PHASE,0,N) * CALC_H(IJK,0,N)

```



```

        VALUE = VALUE + INTERP_WEIGHTS(LC)*FIELD(INTERP_IJK(LC))
    ENDDO
ELSE
! As a safe-guard, if DES_INTERP_ON = .FALSE., return the value of the
! field variable associated with the fluid cell containing the
! particle's center.
    VALUE = FIELD(PIJK(NP,4))
ENDIF
RETURN
END FUNCTION TO_PARTICLE

!-----!
! Function: TO_FIELD - DO NOT EDIT                                     !
!                                                                                   !
! Purpose: Distribute particle effects to Eulerian grid. The provided      !
! scalar values should have the units g/sec. These must be mapped to      !
! the grid by dividing by the cell volume to get g/(cm^3.sec).           !
! .....,.....!
SUBROUTINE TO_FIELD(FIELD, SCALAR)
! Field to be distributed to from particle
    DOUBLE PRECISION, INTENT(INOUT) :: FIELD(DIMENSION_3)
! Value to be distributed
    DOUBLE PRECISION, INTENT(IN) :: SCALAR
! Loop counter
    INTEGER LC

    IF(DES_INTERP_ON) THEN
        DO LC = 1, INTERP_ORDER**DIMN
! Set variable values
! Portion the source term to cell IJK
            FIELD(INTERP_IJK(LC)) = FIELD(INTERP_IJK(LC)) + &
                INTERP_WEIGHTS(LC) * SCALAR / VOL(INTERP_IJK(LC))
        ENDDO ! LC-loop
    ELSE
        FIELD(PIJK(NP,4)) = FIELD(PIJK(NP,4)) + SCALAR/VOL(PIJK(NP,4))
    ENDIF
    RETURN
END SUBROUTINE TO_FIELD

END SUBROUTINE DES_RATES

```

```
! Module name: DES_REACTION_MODEL  
!  
! Purpose:  
!  
! Author: J.Musser Date: 16-Jun-10  
!  
! Comments:  
!  
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!  
SUBROUTINE DES_REACTION_MODEL(NP, FOCUS)  
  
    Use constant  
    Use des_rxns  
    Use des_thermo  
    Use discretelement  
    Use paraml  
  
    IMPLICIT NONE  
  
! Passed variables  
!-----  
! Index value of particle  
    INTEGER, INTENT(IN) :: NP  
! Logical indicating that the specified particle is of special interest  
    LOGICAL, INTENT(IN) :: FOCUS  
  
! Local variables  
!-----  
! index of solids phase and species  
    INTEGER M, N, NN  
! total rate of consumption/production of species (g/sec)  
    DOUBLE PRECISION SUM_DES_R_sc, SUM_DES_Rs  
! masses of species comprising the particle (g)  
    DOUBLE PRECISION S_MASS( DES_NMAX(PIJK(NP,5)) )  
  
    DOUBLE PRECISION PERCENT_REDUCE  
    LOGICAL REDUCED  
    LOGICAL ALL_GONE( DES_NMAX(PIJK(NP,5)) )  
  
    DOUBLE PRECISION, PARAMETER :: P43 = 4.0d0/3.0d0  
    DOUBLE PRECISION DELTA_CORE  
  
    DOUBLE PRECISION dMdt, dXdt, dRdt  
  
! Initialize local variables  
    M = PIJK(NP,5)  
! Return to the calling routine if the species equation for this mass  
! phase is not being solved.  
    IF(.NOT.DES_SPECIES_EQ(M))RETURN  
  
! Check to see if any of the reaction rate will consume more than the  
! available species in the particle.  
    REDUCED = .TRUE.  
    ALL_GONE(:) = .FALSE.  
    DO WHILE(REDUCED)  
! Initialize local variables
```

```

        SUM_DES_Rs = ZERO
        SUM_DES_R_sc = ZERO
! Reset the flag
        REDUCED = .FALSE.
        DO N=1,DES_NMAX(M)
! Calculate the current mass of species N in the particle
            S_MASS(N) = DES_X_s(NP,N) * PMASS(NP)
            IF((S_MASS(N) - DTSOLID*DES_R_sc(NP,N)) < ZERO) THEN
! Flag that the consumption and production rates need reduced
                REDUCED = .TRUE.
! Indicate that the last of the species is gone.
                ALL_GONE(N) = .TRUE.
! Calculate the amount of reduction needed
                PERCENT_REDUCE = S_MASS(N) / (DTSOLID*DES_R_sc(NP,N))
! Reduce the production/consumption rates for each species
                DO NN=1,DES_NMAX(M)
                    DES_R_sc(NP,NN) = DES_R_sc(NP,NN)*PERCENT_REDUCE
                    DES_R_sp(NP,NN) = DES_R_sp(NP,NN)*PERCENT_REDUCE
                ENDDO
            ELSE
! Calculate the total rate of change in particle mass
                SUM_DES_Rs = SUM_DES_Rs + (DES_R_sp(NP,N)-DES_R_sc(NP,N))
! Calculate the total rate of consumption
                SUM_DES_R_sc = SUM_DES_R_sc + DES_R_sc(NP,N)
            ENDIF
        ENDDO
    ENDDO

! Update the particle's mass.
! The mass of the particle is updated first so that it can be used in
! updating the species mass percent of the particle.
!-----
        dMdt = SUM_DES_Rs
        IF (TRIM(DES_INTG_METHOD) .EQ. 'EULER') THEN
! First-order method: Euler
            PMASS(NP) = PMASS(NP) + DTSOLID*dMdt
        ELSEIF (TRIM(DES_INTG_METHOD) .EQ. 'ADAMS_BASHFORTH') THEN
! Second-order Adams-Bashforth scheme
            IF(FIRST_PASS == .TRUE.) THEN
                PMASS(NP) = PMASS(NP) + DTSOLID*dMdt
            ELSE
                PMASS(NP) = PMASS(NP) + DTSOLID * &
                    (1.50d0*dMdt-0.5d0*dMdt_OLD(NP))
            ENDIF
! Store the current value as the old value.
            dMdt_OLD(NP) = dMdt
        ENDIF

! Update the species mass percent
!-----
        DO N=1,DES_NMAX(M)
            IF(.NOT.ALL_GONE(N)) THEN
                dXdt = ((DES_R_sp(NP,N)-DES_R_sc(NP,N)) - DES_X_s(NP,N) * &
                    SUM_DES_Rs)/PMASS(NP)
                IF (TRIM(DES_INTG_METHOD) .EQ. 'EULER') THEN
! First-order method: Euler
                    DES_X_s(NP,N) = DES_X_s(NP,N) + DTSOLID*dXdt
                ELSEIF (TRIM(DES_INTG_METHOD) .EQ. 'ADAMS_BASHFORTH') THEN
! Second-order Adams-Bashforth scheme
                    IF(FIRST_PASS == .TRUE.) THEN
                        DES_X_s(NP,N) = DES_X_s(NP,N) + DTSOLID*dXdt
                    ELSE
                        DES_X_s(NP,N) = DES_X_s(NP,N) + DTSOLID * &

```



```

                (1.50d0*dXdt - 0.5d0*dXdt_OLD(NP,N))
            ENDIF
! Store the current value as the old value.
            dXdt_OLD(NP,N) = dXdt
        ENDIF
    ELSE
        DES_X_s(NP,N) = ZERO
    ENDIF
ENDDO

! Shrinking core model.
!-----
    IF (TRIM(REACTION_MODEL) == 'SHRINKING_CORE') THEN
        IF (SUM_DES_R_sc /= ZERO) THEN
            DOM = 4.0d0*Pi*CORE_Rho(NP)*(CORE_RAD(NP))**2
! Restrict the the size of the denominator to prevent floating point
! issues.
            IF (DOM > 1.0d-6) THEN
! Advance the solution to the core's radius
                dRdt = (-SUM_DES_R_sc)/DOM
                IF (TRIM(DESG_INTG_METHOD) .EQ. 'EULER') THEN
! First-order method: Euler
                    DELTA_CORE = DTSOLID*dRdt
                ELSEIF (TRIM(DESG_INTG_METHOD) .EQ. 'ADAMS_BASHFORTH') THEN
! Second-order Adams-Bashforth scheme
                    IF (FIRST_PASS == .TRUE.) THEN
                        FIRST_PASS = .FALSE.
                        DELTA_CORE = DTSOLID*dRdt
                    ELSE
                        DELTA_CORE = DTSOLID * &
                            (1.5d0*dRdt - 0.5d0*dRdt_OLD(NP))
                    ENDIF
! Store the current value as the old value.
                    dRdt_OLD(NP) = dRdt
                ENDIF
! If the radius will remain positive, update it's value
                IF ((CORE_RAD(NP) + DELTA_CORE) > ZERO) THEN
                    CORE_RAD(NP) = CORE_RAD(NP) + DELTA_CORE
                ELSE
! To prevent the radius from being less than zero, limit value to zero.
                    CORE_RAD(NP) = ZERO
                ENDIF
            ELSE
! To prevent the radius from being less than zero, limit value to zero.
                CORE_RAD(NP) = ZERO
            ENDIF
        ENDIF
! update variables
        RO_Sol(NP) = PMASS(NP)/PVOL(NP)

! Shrinking particle model.
!-----
        ELSEIF (TRIM(REACTION_MODEL) == 'SHRINKING_PARTICLE') THEN
            DES_RADIUS(NP) = (PMASS(NP)/(P43*Pi*Ro_Sol(NP)))** (1.0d0/3.0d0)
! update variables
            PVOL(NP) = PMASS(NP)/Ro_Sol(NP)

! Progressive conversion model
!-----
        ELSEIF (TRIM(REACTION_MODEL) == 'PROGRESSIVE_CONVERSION') THEN
! update variables
            RO_Sol(NP) = PMASS(NP)/PVOL(NP)
        ENDIF

```

```

! Update one over the particle's moment of inertia
  OMOI(NP) = 5.0d0 / (2.0d0 * PMASS(NP) * DES_RADIUS(NP)**2)

! Clear the necessary variables.
  DES_R_sp(NP,:) = ZERO
  DES_R_sc(NP,:) = ZERO

  RETURN
CONTAINS

END SUBROUTINE DES_REACTION_MODEL

```