DEM HEAT TRANSFER MODELS

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Summary

1 – Introduction

Thermomechanical Simulation

Besides mechanical energy, DEM particles can also exchange thermal energy.

Mechanical energy exchange

Leads to the resulting force and torque acting upon a particle, which is responsible for its motion (displacements and rotations)

Thermal energy exchange

Leads to the net heat flux towards or outwards a particle, which is responsible for its temperature variation

This presentation covers heat transfer models for soft-sphere DEM, considering round-shaped particles (2D discs or 3D spheres)

Lumped Capacitance Analysis

Biot number

Dimensionless number that gives the ratio of the heat transfer resistance by conduction inside the body and by convection on its surface:

$$Bi = \frac{h_i l_i}{k_i}$$

It quantifies the relative importance of conduction and convection to determine whether or not the inner temperature vary significantly in space while it is heated or cooled from a thermal gradient applied to its surface.

Isothermal particles

Valid assumption for thermally thin bodies, in which the *Biot* number is much smaller than unity ($Bi < 0.1$) and the thermal resistance within particles can be neglected.

In this case, heat conduction inside the particle is much faster than heat transfer across its surface, so the thermal gradient is negligible and the temperature can be considered as uniform within each particle (Holman, 1981; Incropera, 2006, Cengel, 2007).

small Biot number

uniform particle temperature

large Biot number

temperature gradient inside the particle
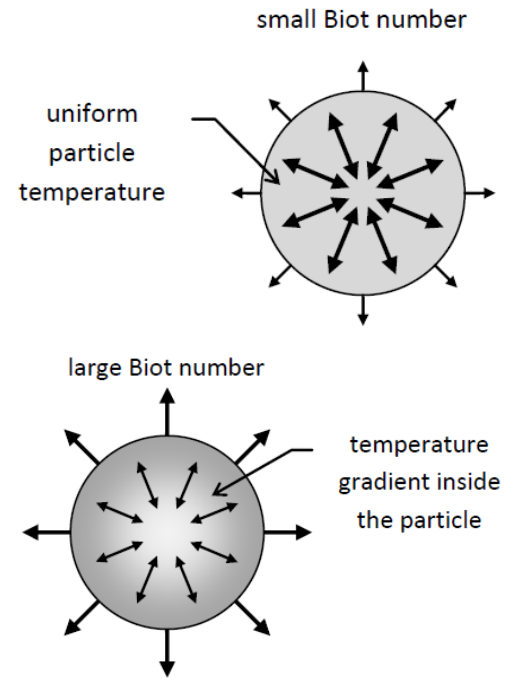
Musser (2011)

Time Step Calculation Cycle

The equations of Newton's 2nd law to obtain the motion of particles remain unchanged, and an additional equation for energy conservation (1st law of thermodynamics) needs to be solved simultaneously to obtain the temperature variation of each particle.
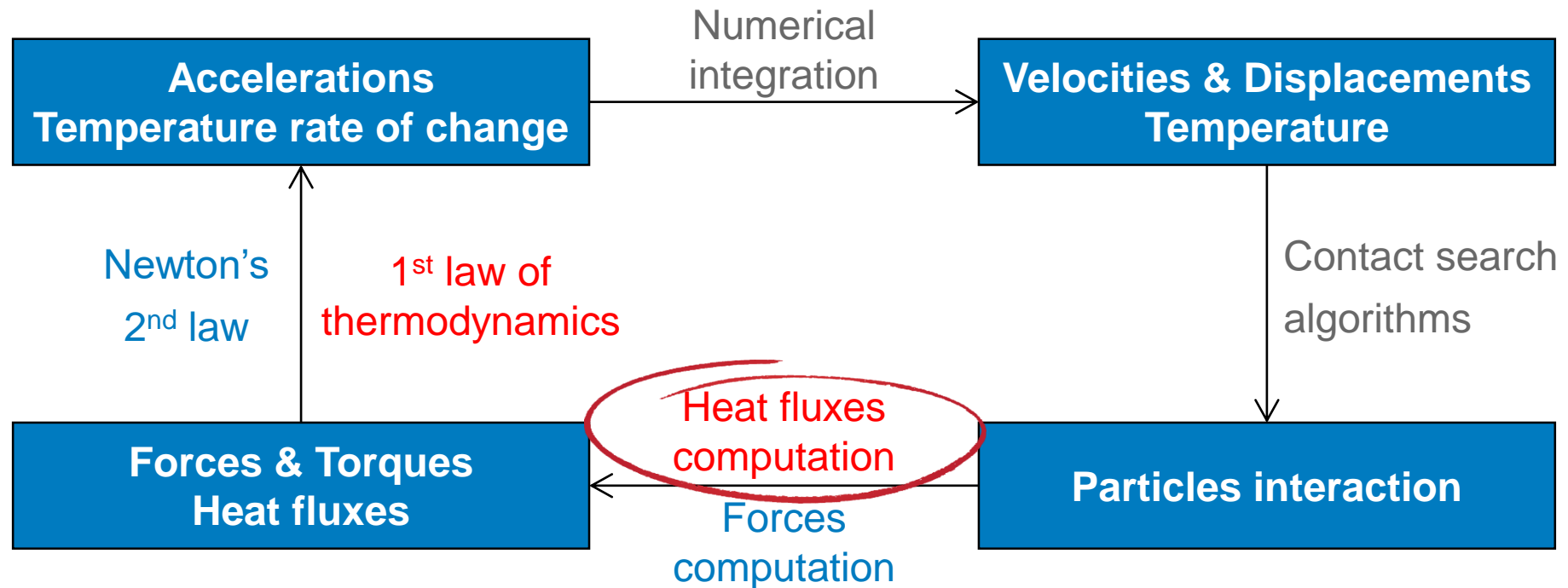
Temperature Calculation

Unsteady equation of energy conservation: $m_i c_i \dfrac{dT_i}{dt} = Q_i$
(from the 1st law of thermodynamics)

Temperature rate of change: $\dfrac{dT_i}{dt} = \dfrac{Q_i}{m_i c_i}$

Numerical integration: $\dfrac{dT}{dt} = \dfrac{T^{t+\Delta t} - T^t}{\Delta t}$
(forward Euler scheme)

Temperature evolution: $T_i^{t+\Delta t} = T_i^t + \dfrac{Q_i^t}{m_i c_i} \Delta t$

Target:
Determine the net rate of heat transferred to each particle in each time step (Q_i^t)!

Initial condition: $T_i(t = 0) = T_i^0$

Coupled Problem

Thermomechanical coupling

The equations of motion and energy conservation are coupled because heat fluxes depend on the kinematics (positions, velocities, etc.), and the mechanical properties can also depend on the temperature.

Coupling scheme

In each time step, the mechanical and thermal problems are solved simultaneously with the position, velocity and temperature from the previous time step.
The mechanical and thermal problems are decoupled within a single time step, so that the solution of one physics does not affect the other during one step.
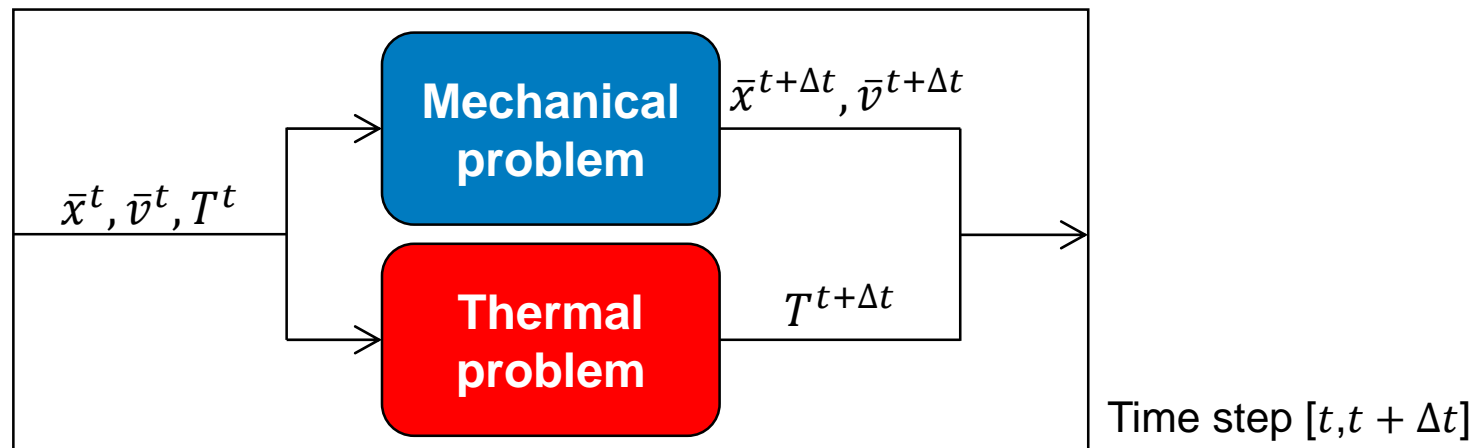
Time Step Size

Quasi-steady temperature criterion

The size of the time step must be such that the temperature of each particle changes slowly enough so that thermal disturbances do not propagate further than its immediate neighbors during one time step, as with the elastic waves in the mechanical problem (Vargas & McCarthy, 2001).

However, the time step condition for the thermal problem is much less restrictive than for the mechanical problem, hence by ensuring the time integration stability for the mechanical problem automatically ensures the stability for the thermal problem.

The critical time step for the stability of the explicit time integration scheme for the solution of the thermal problem can be estimated by the critical value for the one-dimensional heat conduction problem (Cengel, 2007).

Critical time step of thermal problem: (Rojek, 2014)

$$\Delta t_{\mathrm{cr}} = \frac{\rho c R}{k}$$

Critical time step of mechanical problem: (Li et al, 2005)

$$\Delta t_{\mathrm{cr}} = \frac{\pi R \sqrt{\rho/G}}{0.8766 + 0.163 \nu}$$

Each particle provides a different value for Δt_{cr}, so the minimum should be considered

Heat Transfer Mechanisms

In the presence of a temperature gradient, heat can be transferred by 3 mechanisms: **conduction**, **convection**, **radiation**.

In <u>fluid-filled packed beds</u>, these mechanisms are identified by (Yagi & Kunii, 1957):

1. **Conduction** within particles
   (i.e. non-isothermal particles)
2. **Conduction** between fluid in adjacent voids
   (i.e. within the fluid)
3. **Conduction** between particles
   (contacted or non-contacted particles)
4. **Convection** between fluid and particles
5. **Convection** within the fluid
6. **Radiation** between particles' surfaces
   (in case of interstitial gas)
7. **Radiation** between fluid in adjacent voids
   (in case of interstitial gas)
8. **Radiation** between fluid and particles
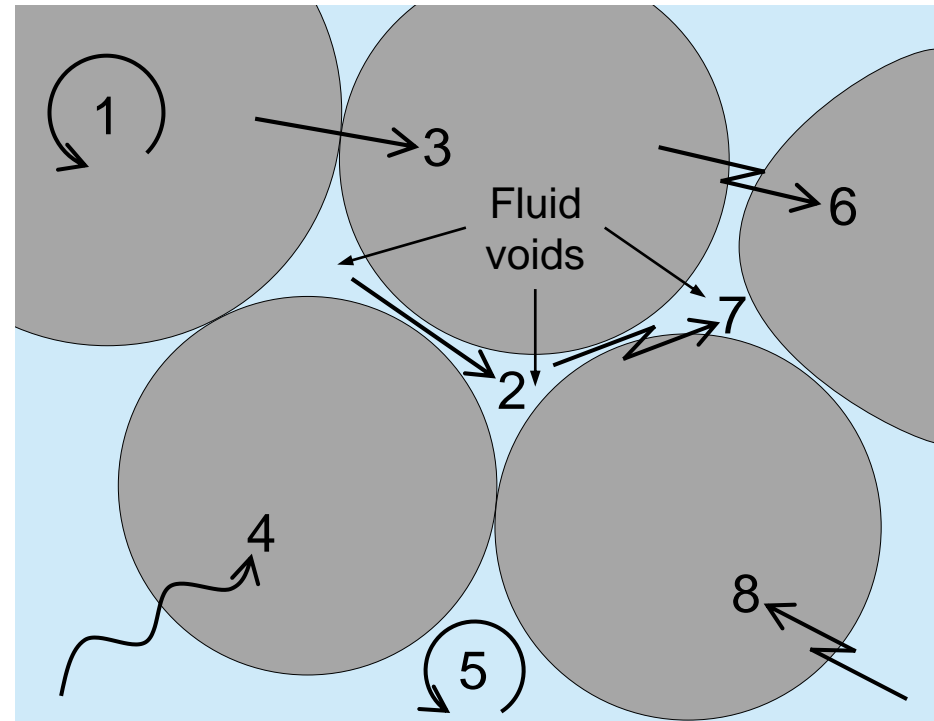
Most DEM simulations only deal with the mechanisms involving the particles. Solving the fluid phase behavior would require a coupled DEM-CFD solution. Focus here on relevant mechanisms for <u>tracking particles temperature</u> (3,4,6).

Mechanism 2: Cheng et al, 2020

Heat Transfer Mechanisms

Typical components of the net rate of heat transferred to a particle
(positive direction of heat transfer is "entering" the analyzed body – particle i):
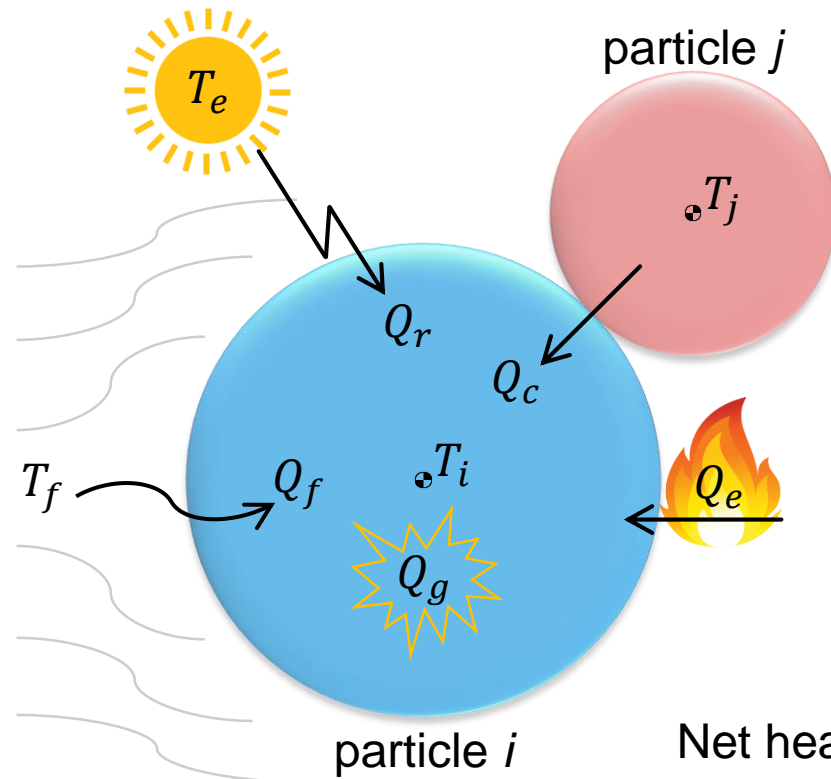
$Q_c \rightarrow$ **Conduction** with neighboring objects
(particles and walls: temperature T_j)

$Q_f \rightarrow$ **Convection** with surrounding fluid
(temperature T_f)

$Q_r \rightarrow$ **Radiation** with surrounding environment
(temperature T_e)

$Q_g \rightarrow$ Heat **generation**
(energy dissipation, chemical reaction, etc)

$Q_e \rightarrow$ Heat **source**
(fire nozzles, burners, laser beams, etc)

Net heat rate: $Q_i = \sum Q_{c,ij} + Q_{f,i} + Q_{r,i} + Q_{g,i} + Q_{e,i}$

Not all of these mechanisms exist or need to be considered in a specific problem.

Motion of Granular Materials

According to Campbell (2006), all the important granular flows are dense, which means that the particles are constantly in contact with each other, either in a static way or through long-lasting collisions.

However, dilute flows where particle collisions are shorter and less frequent cannot be ignored in the study of heat transfer, as they are part of some industrial application.
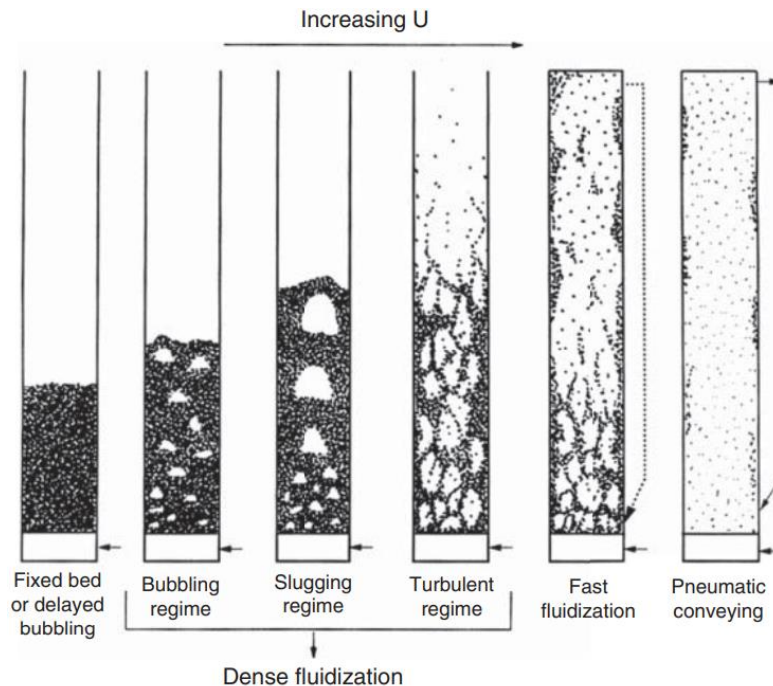
Crowe (2006)

For example, in fluidized reactors, depending on the inlet fluid velocity, different regimes might be observed for the granular bed, ranging from a packed bed with no particle motion to a fluidized regime with much less particle contacts.

To account for the fluid motion and temperature, CFD-DEM coupling strategies has been widely used in the study of particle-fluid flow, which is also referred to as Eulerian-Lagrangian methods, but many other coupling strategies can be employed for multiphase flows (Zhu et al, 2007; Wang et al, 2019).

Influence of different heat transfer mechanisms

Zhou et al (2009):
Performed CDF-DEM simulations of **packed and fluidized beds**, by using different velocities for the in-flowing gas. The increase of the gas velocity makes the contribution from fluid convection to increase and the conduction to decrease. Under the low temperature conditions (373K), the radiative contribution is very low.

Figure 14. Bed-averaged convective, conductive and radiative heat transfer coefficients (calculated according to Eq. 20a, c and d, respectively) as a function of gas superficial velocity.

Yang et al (2015):
Performed CDF-DEM simulations of heat transfer in **moving beds** with an inlet gas accounting for conduction, convection and radiation. It shows that particle-fluid convection is dominant with the conduction being much lower and radiation almost insignificant for the considered temperature (although becoming important at higher temperatures).
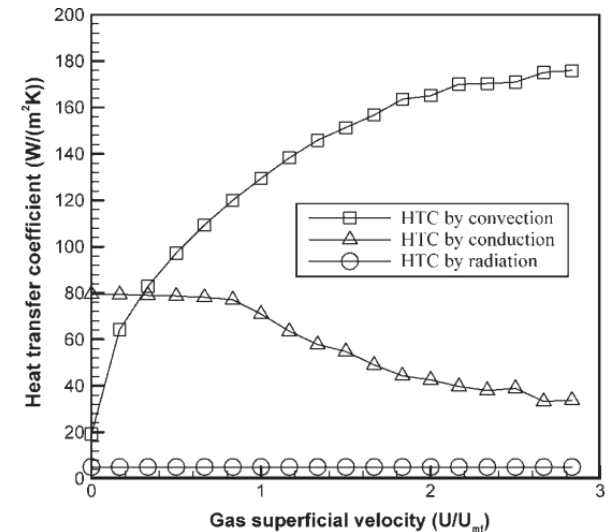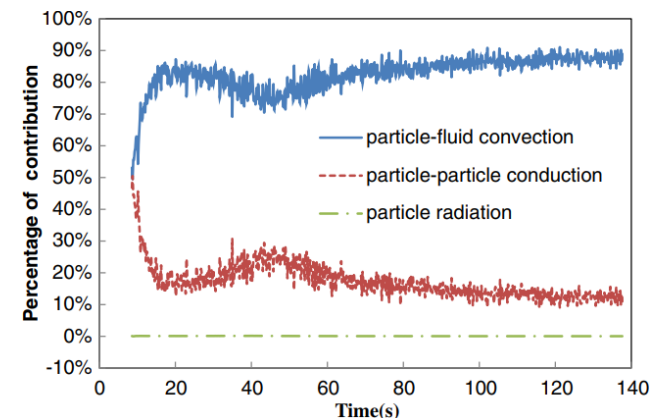
Influence of different heat transfer mechanisms

Lu et al (2017):
Performed coarse grained CFD-DEM simulations of heat transfer in **fluidized beds**, neglecting radiation. Particle-fluid convection accounts for about 65% of the total heat loss while the rest is mainly caused by particle-fluid-wall conduction. The particle-wall contact conduction accounts for less than 1%.
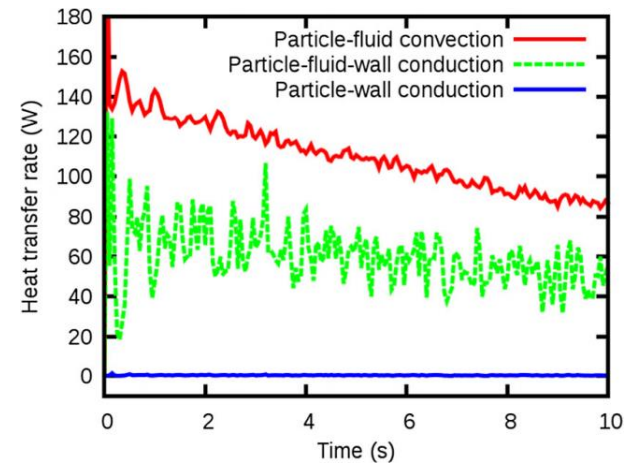
Wang et al (2019):
Performed CFD-DEM simulations of heat transfer in **fluidized beds**, neglecting radiation. The particle-fluid convection dominates the heat transfer while the particle-particle conduction is almost negligible and the particle-fluid-particle conduction occupies about 10% of the total heat transfer.

2 – Conductive Heat Transfer

Conductive Heat Transfer

Conductive heat transfer between particles can occur by different mechanisms (Yagi & Kunii, 1957; Cheng et al, 1999):

Direct conduction
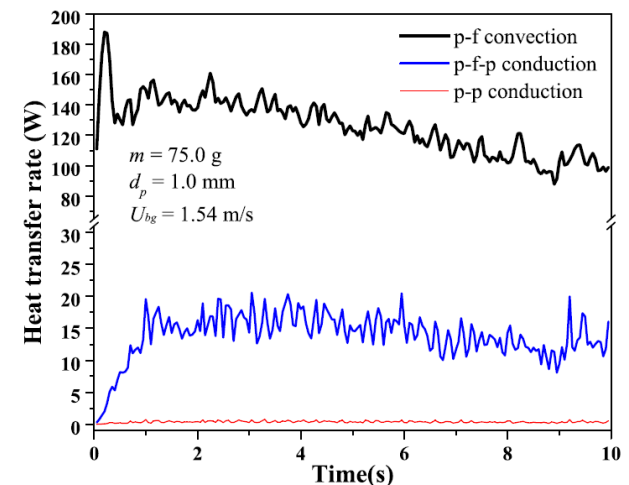
Heat conduction through the contact area of two touching particles (contact particle-particle, Q_{cpp})

Indirect conduction

Heat conduction through the fluid in-between two touching particles (contact particle-fluid-particle, Q_{cpfp}), or non-touching particles that are very close (non-contact particle-fluid-particle, Q_{npfp})

The total heat conduction of touching particles is given by the sum of Q_{cpp} and Q_{cpfp}.
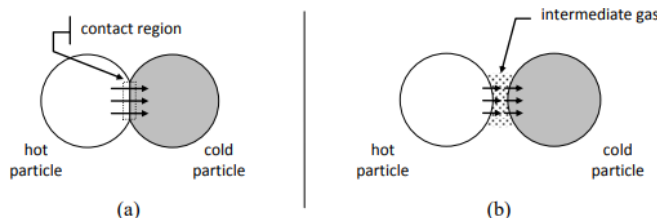
Figure 3-1: Illustration of conduction between particles. (a) *Contact conduction*: thermal energy is transferred from a hot particle to a cold particle through their shared contact area. (b) *Particle-fluid-particle conduction*: thermal energy is transferred from a hot particle to the stagnant gas separating its surface from the cold particle. The thermal energy is then transferred from the stagnant gas to the cold particle.

Musser (2011)
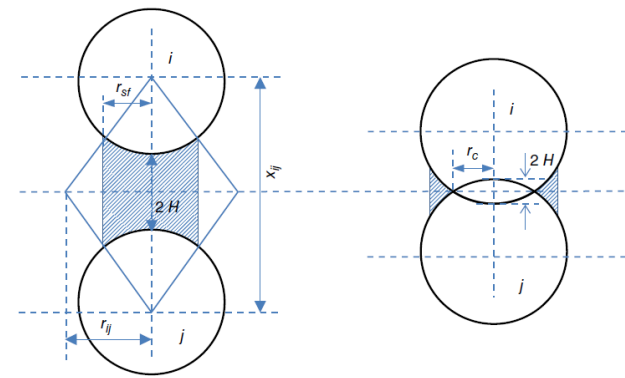
Zhou et al (2009)

Conductive Heat Transfer

According to Zhou et al (2009), the contribution of each conduction mechanism in <u>packed and fluidized beds</u> is:

- **Non-contact particle-fluid-particle** (triangle):

In fluidized beds (x-axis > 1), this mechanism is more relevant than the others for most values of the thermal conductivity of particles.

- **Contact particle-fluid-particle** (circle):

In fixed beds (small values of x-axis), this mechanism is more relevant than non-contact particle-fluid-particle for most values of the thermal conductivity of particles.

- **Contact particle-particle** (square):

Irrelevant for low thermal conductivity of particles (< 1%). For high thermal conductivity, its importance is relevant but decreases from fixed to fluidized beds.
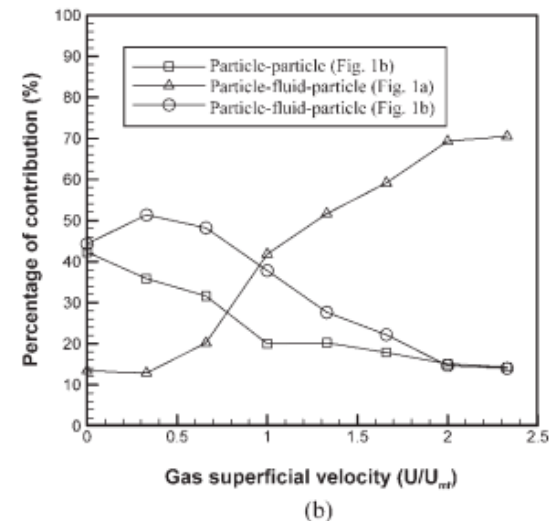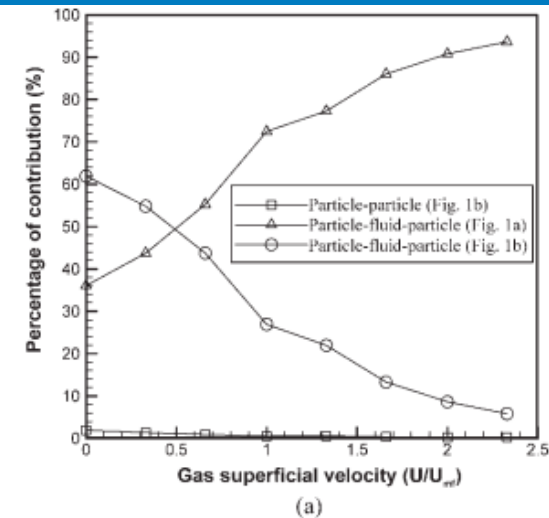
Figure 12. Contributions to conduction heat transfer by different heat transfer mechanisms under the condition of (a) $k_p = 0.08$ W/(m·K), and (b) $k_p = 30$ W/(m·K).

According to Zhou et al (2010) the contribution of each conduction mechanism to the total conduction heat transfer in <u>packed beds with stagnant fluid in-between</u> is described as:

For low thermal conductivity of particles, relative to the interstitial fluid, Q_{cpfp} is dominant. As particle conduction increases, both particle-fluid-particle mechanisms weakens and Q_{cpp} becomes more significant. For high thermal conductivities of particles, Q_{cpp} becomes dominant, but Q_{cpfp} is still important.
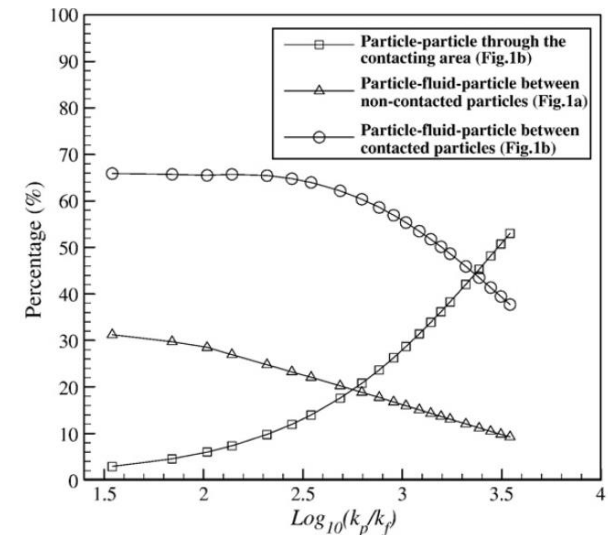
Fig. 8. Relative contributions of the heat transfer mechanisms to the overall heat transfer under the base condition (note: the percentage is the ratio of each heat flux to the total heat flux under the thermal equilibrium condition).

It was also observed that the relative importance of each conduction mechanism to the total conduction heat transfer is insensitive to the bed temperature, for low or high thermal conductivity of particles (although the total conduction contribution decreases in high temperature, as radiation contribution increases).

Conductive Heat Transfer

Similarly, according to Cheng et al (1999) the contribution of each conduction mechanism to the total conduction heat transfer in <u>packed beds with a stagnant fluid</u>, is observed as:

- **Non-contact particle-fluid-particle** (line 1):

Contribution is relatively low for most values of the ratio between particle and fluid thermal conductivities (referred to as k_p/k_f).

- **Contact particle-fluid-particle** (line 2):

Dominant when k_p/k_f is low.

- **Contact particle-particle** (line 3):

Becomes important when k_p/k_f increases.
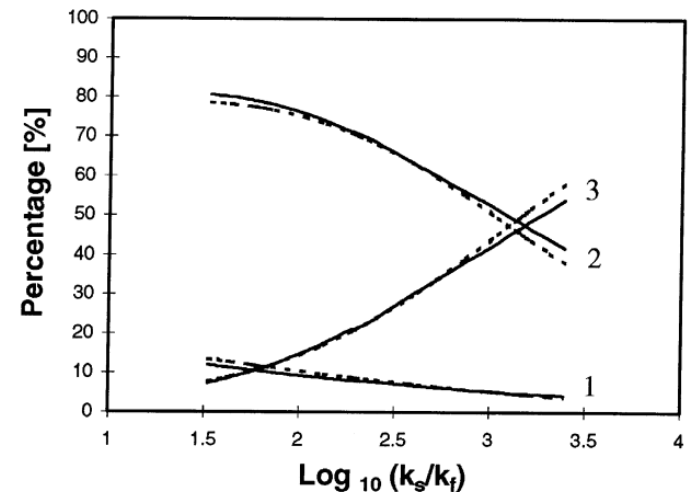
Fig. 11. Relative contributions of the heat transfer mechanisms to the overall heat transfer: line 1, the conduction through the solid particles and stagnant fluid between non-contacted particles; line 2, the conduction through the solid particles and stagnant fluid between contacted particles; and line 3, the conduction through the contact area between contacted particles; (——), Model A; (- - -), Model B ($c = 0.5$).

It was also shown that the relative importance of different conduction mechanisms may vary for different packing structures, so these conclusions may be affected by the particle size distribution, shapes, etc. (e.g. ellipsoids are analyzed in Gan et al, 2016).

Conductive Heat Transfer

Remarks from literature – Systems with static contacts

Batchelor & O'Brien (1977)

Contact particle-particle conduction dominates in packed beds when the interstitial medium is stagnant and composed of a material whose thermal conductivity is small compared to the particles ($k_p R_c / k_f R_p \gg 1$)

Vargas (2002)

The main heat transfer mechanism under packed and vacuum conditions is conduction through the contact surface of the particles

Molerus (1997)

If k_p / k_f is high, the contact conductance between adjacent particles is the controlling process in both static and slowly moving beds of particles, in the presence of a stagnant interstitial gas

Morris et al (2015)

Particle–fluid-particle conduction is significant in systems where $k_p R_c / k_f R_p > 1$

Wakao & Kato (1969)

Heat conduction between particles is known to be dominant in packed beds with high k_p / k_f (>10)

Chen et al (2019)

The solid contact conduction, solid-fluid-solid conduction, and radiation are considered in the thermal DEM model as the main heat transfer mechanisms in packed beds with stagnant fluid

Zhou et al (2009)

In fixed beds, the conduction is dominant for high thermal conductivities of particles due to the large heat flux through the contact area

Morris et al (2016)

The significance of particle-particle heat transfer relative to particle-fluid-particle conduction depends on $k_p R_c / k_f R_p$: when it is less than one, indirect conduction is dominant. For example, in sand the indirect conduction was observed as two orders of magnitude larger than the direct mechanism.

Botterill et al (1989)

Heat conduction between particles is known to be dominant for packed beds with stagnant fluid at low temperatures (< 450K)

Schlunder (1980)

Concluded that the mechanism of heat transfer at medium and long contact times is different to that at very short contact times

Quintana-Ruiz & Campello (2020)

Heat transfer in dry particle systems is often regarded to occur mostly through conduction

Conductive Heat Transfer

Remarks from literature – Systems with particles collision

Sun & Chen (1988)
The collisional conduction is not a dominant mechanism in fluidized bed under typical conditions (it is negligible)

Li & Mason (2000), Schlunder (1982)
Heat conduction during the collision between particles must be included in dense flows, where particles are frequently in contact with their neighbors

Morris et al (2016a)
Particle-particle and particle–fluid–particle conductions can be neglected for many dilute systems because contacts are infrequent and durations are short.
In moderate-to-dense particle flows, enduring contacts are frequent and conduction between particles is significant.

Saxena et al (1979)
Heat conduction during the collision between particles may be neglected in dilute flows

Vargas (2002)
Contact conduction during collisions is the dominant heat transfer mechanism in dense slow flowing systems

Moysey & Thompson (2005)
Since thermal conductivity of the solid particles is much greater than that of the stagnant interstitial medium, only heat transfer between particle contacts is considered in dense flow

Fan & Zhu (1998)
Typically, heat transfer as a result of particle-particle and particle-wall contact is assumed negligible in gas-solids systems due to small contact area and short contact time

Lu et al (2017)
In fluidized beds, the total conduction contribution is about 1/4 of the convection, thus the particle-particle conduction accounts for a very small fraction of the total heat transfer, even for high thermal conductivity values

Peng et al (2020)
In particulate flows with an average solid concentration > 0.2, a large number of collisions occur concurrently, resulting in a significant amount of heat energy transferred through conduction through collisional contacts, which needs to be considered.

Direct Conduction

Two types of heat transfer due to contact particle-particle conduction are identified:

Collisional contact conduction

Applicable to systems in which particles are moving and colliding against each other or against walls, i.e. contacts last for a very short time
(e.g. moving and fluidized beds, etc).

Static contact conduction

Applicable to systems in which particles are in static contact, i.e. there is a permanent contact and they keep in touch with no relative velocity
(e.g. fixed / packed beds, granulators, etc).

As suggested by Zhou et al (2009), in fixed beds all contacts are static and only the static regime applies. In fluidized beds, although contact conduction seems negligible, both regimes can be considered as follows:

- Collisional contact conduction is used while the contact time is lower than the expected collisions time (t_c).

- Static contact conduction is used after the contact time surpasses the expected collision time (t_c).

Direct Conduction

Model by Sun & Chen (1988)

Numerical and theoretical analysis of transient heat conduction <u>due to particle collision</u>, as a quantitative evaluation of the concepts initially presented by Soo (1967).

Elastic collisions based on <u>Hertz theory</u> and no thermal resistance between surfaces.

Heat conduction assumed to be similar to that between two semi-infinite media.

Small Fourier number: 1D heat flow is assumed and an analytical solution is obtained. High Fourier number: a correction factor is employed based on numerical simulations.

The semi-infinite media assumption is inaccurate for large thermal conductivities of particles (overestimates the heat transfer when Fourier number is high).

Total thermal energy exchanged during impact:

$$U = C \frac{0.87\pi (R_c^{\max})^2 t_c^{1/2}}{(\rho_i c_i k_i)^{-1/2} + (\rho_j c_j k_j)^{-1/2}} (T_j - T_i)$$

where C is a correction factor obtained by numerical computation (provided in graphs).

The rate of heat transfer may be obtained by:

$$Q_{cpp} = U/t_c$$

Direct Conduction

Model by Zhou et al (2008)

FEM is employed to simulate the transient heat conduction between <u>colliding spheres</u>, assuming elastic collisions based on <u>Hertz theory</u>.

Improved the equation of Sun & Chen (1988) to fit the FEM results.

Small Fourier number: the new equation is consistent with the analytical results of the semi-infinite media assumption of Sun & Chen (1988).

High Fourier number: the new equation solves the overestimation issue of the semi-infinite media assumption (besides not depending on a non-practical factor).

The new equation still overestimates the heat flux when the particle conductivities are significantly different, and it is not recommended for temperature dependent properties.

Rate of heat transfer:
$$Q_{cpp} = C \frac{\pi (R_c^{\max})^2 t_c^{-1/2}}{(\rho_i c_i k_i)^{-1/2} + (\rho_j c_j k_j)^{-1/2}} (T_j - T_i)$$

Direct Conduction

Model by Zhou et al (2008)

In the previous equation:

$$C = 0.435 \left(\sqrt{C_2{}^2 - 4C_1(C_3 - F_o)} - C_2 \right)/C_1$$

$$C_1 = -2.300\left(\rho_i c_i / \rho_j c_j\right)^2 + 8.909\left(\rho_i c_i / \rho_j c_j\right) - 4.235$$

$$C_2 = +8.169\left(\rho_i c_i / \rho_j c_j\right)^2 - 33.770\left(\rho_i c_i / \rho_j c_j\right) + 24.885$$

$$C_3 = -5.758\left(\rho_i c_i / \rho_j c_j\right)^2 + 24.464\left(\rho_i c_i / \rho_j c_j\right) - 20.511$$

Fourier number: $F_o = \dfrac{\alpha_i t_c}{l_i{}^2} = \dfrac{k_i t_c}{\rho_i c_i (R_c^{\max})^2}$

Direct Conduction

Model by Batchelor & O'Brien (1977)

Studied the steady-state thermal flux between two smooth-elastic particles pressed together by a <u>static compression</u> load forming a flat circle of contact, considering the <u>Hertz theory</u>.

Assumed that particles are in vacuum, thus valid for high values of k_p/k_f.
In this condition, the approximately analytical solution of conductive heat transfer is:

$$Q_{cpp} = 2k_p R_c^{\mathrm{htz}}\left(T_j - T_i\right)$$

Other models have been developed (Siu & Lee, 2004; Feng et al, 2008; Sridhar & Yovanovich ,1996; Lambert & Fletcher,1997; Chan & Tien, 1973) but this one is simple and matches experimental data for conduction through packed beds reasonably well.

Used by many authors in different applications to compute heat transfer by conduction during static contact (Zhou et al, 2009), or even in moving systems of dense flows (e.g. Vargas & McCarthy, 2001; Chaudhuri et al, 2006; Amritkar et al, 2014, Lu et al, 2017; Moysey & Thompson, 2005, Musser, 2011, etc).

Direct Conduction

Model by Batchelor & O'Brien (1977)

Modification for the contact between particles with different thermal conductivities, using an <u>effective conductivity</u> parameter (Cheng et al, 1999):

$$Q_{cpp} = 4\bar{k}R_c^{\text{htz}}(T_j - T_i)$$

Generalization to consider the contact radius based on the <u>overlap geometry</u>, instead of the radius obtained from the Hertz contact model using the current normal force (Musser, 2011):

$$Q_{cpp} = 4\bar{k}R_c^{\text{geo}}(T_j - T_i)$$

This generic modified formula results in a contact area representative of any contact model and promotes greater modeling consistency, although the contact area may still need a correction due to the use of a <u>low stiffness</u> in the simulation.

Thermal pipe models

Heat is exchanged through a "thermal pipe" connecting the center of touching particles, which behave like heat reservoir (due to the lumped capacitance assumption).

Assumes the discrete form of Fourier law for the heat transfer, and the thermal resistance of the pipe may be considered in different ways.

Suited for modeling continuous materials (Jebahi et al, 2015; Hahn et al, 2011).
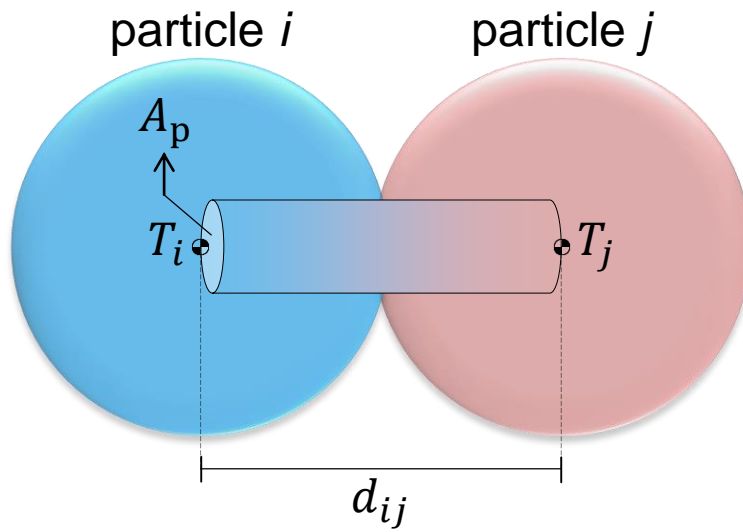
$$Q_{cpp} = \frac{kA_\mathrm{p}}{d_{ij}}\left(T_j - T_i\right)$$

Thermal pipe model by Quintana-Ruiz & Campello (2020)

Simple model for quantifying the contact heat flow under static and dynamic behavior.

$$Q_{cpp} = \frac{\tilde{k} A_p}{d_{ij}}(T_j - T_i) \qquad \text{where} \qquad \tilde{k} = (R_i + R_j)\left(\frac{R_i}{k_i} + \frac{R_j}{k_j}\right)^{-1} \qquad A_p = \pi\left(R_c^{\text{geo}}\right)^2$$

Thermal pipe model by Rojek (2014)

DEM is used for rock modeling, but as a discretization method and not to represent separate particles that come into contact.

$$Q_{cpp} = \frac{k_p A_p}{d_{ij}}(T_j - T_i) \xrightarrow[\;d_{ij} = 2\bar{r}\;]{A_p = 2\bar{r}b} Q_{pp} = k_p b(T_j - T_i)$$

Fig. 10 Equivalence of two particles to a bar in a heat conduction problem

2D model: *b* is assumed as unity.

3D model: *b* is assumed as $\bar{r}$.

$$\bar{r} = \frac{R_i + R_j}{2}$$

Low stiffness correction

In DEM simulations, it is common to use a low value of Young modulus, compared to the real value, to allow larger time steps and decrease computational time.

It usually does not affect much the kinematics of the particles (Morris et al, 2016a).

However, it leads to a larger contact area and collision time, which increases the contact heat transfer.

Some correction factors have been developed to mitigate this problem and allow the use of low a Young modulus while obtaining realistic heat transfer values.

Nevertheless, other problems can arrive from low stiffness of particles, such as the change in porosity distribution.

Morris et al (2016a)

Analytic scaled temperature rise (Eq. 7) vs. a dimensionless thermal relaxation time for a particle resting on a heated surface.

The level of softening is indicated by value H_{sim}/H_{actual}; $H_{sim}/H_{actual} = 1$ refers to non-softened case.
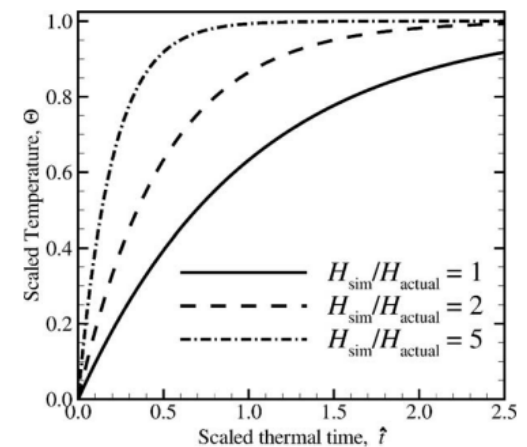
Direct Conduction

Correction by Zhou et al (2010)

Proposed a correction coefficient of the maximum contact radius based on the real and adopted values of the Young modulus.

The coefficient is based on the maximum contact area of Hertz theory for an elastic collision between two spheres.

The reduced contact radius is expressed as:

$$R_c^{\mathrm{cor}} = \left(\frac{\bar{E}}{\bar{E}_{\mathrm{real}}} \right)^{1/5} R_c^{\mathrm{max}}$$

Where $\bar{E}_{\mathrm{real}}$ is calculated as $\bar{E}$ but with real value of Young modulus.

It has been reported to work for both packed and fluidized beds.

The reduced radius is then used in the formulas of contact particle-particle conduction, in place of the overestimated contact radius.

Direct Conduction

Correction by Lu et al (2017)

The correction coefficient of Zhou et al (2010), based on Hertz theory, has been extended to the linear spring-dashpot model.

The reduced contact radius is expressed as:

$$R_c^{\mathrm{cor}} = \left(\frac{K_n R_c}{K_{HZ,\mathrm{real}}} \right)^{2/3}$$

Where k_n and $k_{HZ,\mathrm{real}}$ are, respectively, the normal spring constant used in the simulation and the spring constant derived from the real value of the Young modulus (see appendix A, for the expression of K_{HZ}).

The reduced radius is then used in the formulas of contact particle-particle conduction, in place of the overestimated contact radius.

Direct Conduction

Correction by Morris et al (2016a)

Two correction factors to adjust both the overestimated contact area and contact time.

Based on the Batchelor & O'Brien (1977) model ($Q_{pp} = 2k_p R_c^{\text{htz}} \Delta T$), by applying both correction coefficients:

$$Q_{cpp} = 2k_p \left(\frac{F_n \bar{R}}{\bar{E}_{\text{real}}} \right)^{1/3} \left(\frac{t_{c,\text{real}}}{t_c} \right)^{2/3} \left(T_j - T_i \right)$$

$$\underbrace{\phantom{\left(\frac{F_n \bar{R}}{\bar{E}_{\text{real}}} \right)^{1/3}}}_{\text{area correction}} \quad \underbrace{\phantom{\left(\frac{t_{c,\text{real}}}{t_c} \right)^{2/3}}}_{\text{time correction}}$$

Where F_n and t_c are computed according to the contact law, and $\bar{E}_{\text{real}}$ and $t_{c,\text{real}}$ are computed with the real values of the material properties.

In static systems, the time correction term (ratio of collision times) is equal to unity, and only the area correction term is applied.

This correction performs well for moderately dense flows, but for dense flows it is not recommended as the time correction was derived for a binary collision.

Indirect Conduction

In addition to direct contact conduction (Q_{cpp}), particles may also exchange heat indirectly by the conduction through the thin wedge of interstitial fluid separating their surfaces when they are in close proximity or in contact to one another.

This heat conduction mechanism (now generally referred to as Q_{pfp}) is specially important in scenarios where the thermal conductivity of the fluid is comparable to that of the particles (i.e. $k_p R_c / k_f R_i \gg 1$ is not satisfied).
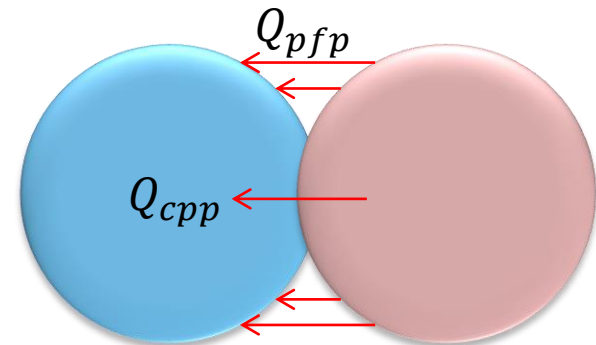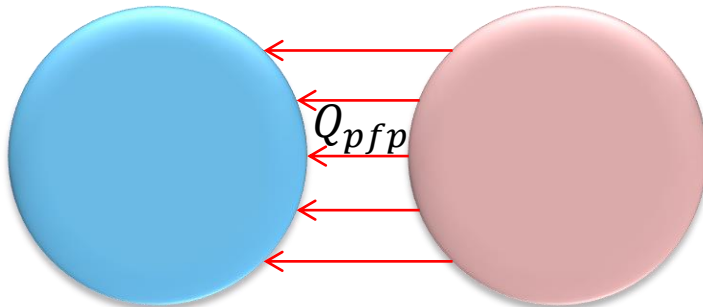
The particle-fluid-particle heat conduction has been studied by several investigators (e.g. Wen & Chang, 1967; Delvosalle & Vanderschuren, 1985; Tsory et al, 2013), but two approaches stand out in the literature:

Voronoi polyhedron methods   **Surrounding layer method**

Voronoi polyhedron methods

Introduced by Cheng et al (1999), with sub-models A and B, for a packed bed with mono-sized particles in the presence of a stagnant fluid. Later modified by Gan et al (2016) and Chen et al (2019) for multi-sized particles.

May require a Voronoi tessellation (Voronoi, 1908) at each time step: time consuming.

Heat transfer between two neighboring particles is restricted to the region delineated by the double pyramid that share a Voronoi boundary plane (including particles' body).

To get an analytical solution, the double pyramid is replaced by a double tapered cone of the same area A_n (of radius r_{ij}) and distance between vertexes (particles centers).
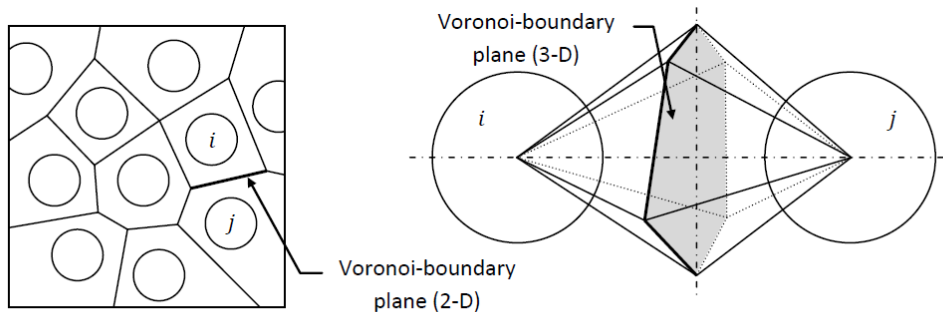
Figure 3-11: The model of Cheng, Yu, and Zulli [65] restricts particle-fluid-particle conduction to the region delineated by the double pyramid (3-D) generated by the Voronoi-boundary plane.

Musser (2011)
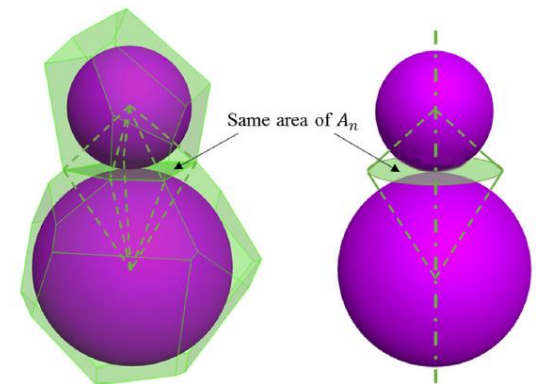
Chen et al (2019)

Voronoi polyhedron – Method A

- The surface of the double tapered cone is isothermal.

- Conduction is negligible in the outer region of the cone (region "B").

- The heat flow paths are parallel to the axis joining the particles' centers.

These assumptions lead to an integral expression for the rate of heat transfer, which needs to be solved numerically by a quadrature.
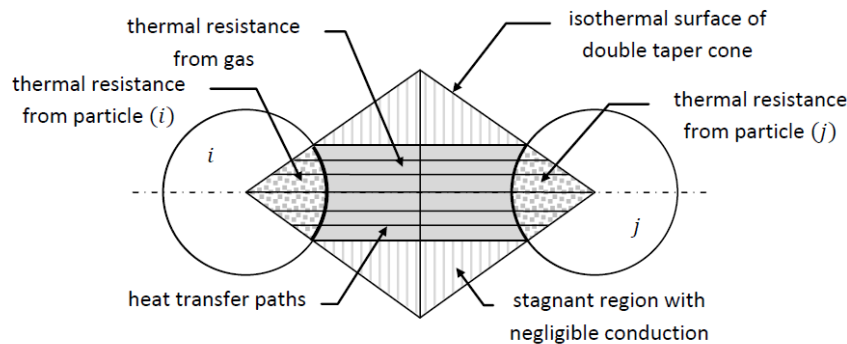
Figure 3-12: Cheng, Yu, and Zulli's [65] *Model A* for particle-fluid-particle conduction assumes that the surface of the double tapered cone is isothermal, conduction is negligible in the outer region of the double tapered cone, and the heat transfer paths are parallel to the axis joining the particles' centers.
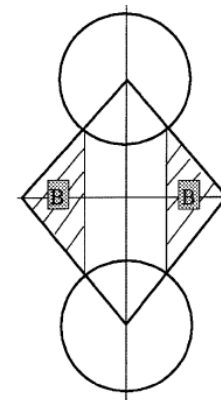
(b) A double taper cone model with shaded area as region B

Musser (2011)

Cheng et al (1999)

Voronoi polyhedron – Method A (mono-size)

For mono-sized particles of radius R_p, Cheng et al (1999) determined that the particle-fluid-particle heat transfer rate by conduction can be obtained from:

$$Q_{pfp} = (T_j - T_i) \int_{R_c}^{r_{sf}} \frac{2\pi r}{\frac{1}{\bar{k}}\left(\sqrt{R_p{}^2 - r^2} - \frac{d_{ij}r}{2r_{ij}}\right) + \frac{1}{k_f}\left(d_{ij} - 2\sqrt{R_p{}^2 - r^2}\right)} dr$$

where: $\quad r_{ij} = \sqrt{\frac{3V_{ij}}{\pi d_{ij}}} \quad\quad r_{sf} = \frac{R_p r_{ij}}{\sqrt{r_{ij}{}^2 + (d_{ij}/2)^2}}$

V_{ij} is the volume of the Voronoi polyhedron (i.e. the double tapered cone) between particles, which is actually the only parameter that depends on the Voronoi tessellation.

When particles are not in contact, $R_c = 0$.

Voronoi polyhedron – Method A (mono-size)

$r = r_{ij}$ (radius of tapered cone)

$\sqrt{r_{ij}^2 + (d_{ij}/2)^2}$

$\dfrac{d_{ij}r}{2r_{ij}}$ d_p d_f d_p $\dfrac{d_{ij}r}{2r_{ij}}$

$r = r_{sf}$

R_p R_p

$r = R_c$

$r = 0$

$r_{sf} = \dfrac{R_p r_{ij}}{\sqrt{r_{ij}^2 + (d_{ij}/2)^2}}$

$\sqrt{R_p^2 - r^2}$ d_f $\sqrt{R_p^2 - r^2}$

$Q_{pfp} = \displaystyle\int_{R_c}^{r_{sf}} dQ$

$d_p(r) = \sqrt{R_p^2 - r^2} - \dfrac{d_{ij}r}{2r_{ij}}$

d_{ij}

$dQ = (T_j - T_i)\dfrac{2\pi r}{\dfrac{2d_p}{k_p} + \dfrac{d_f}{k_f}} dr$

$d_f(r) = d_{ij} - 2\sqrt{R_p^2 - r^2}$
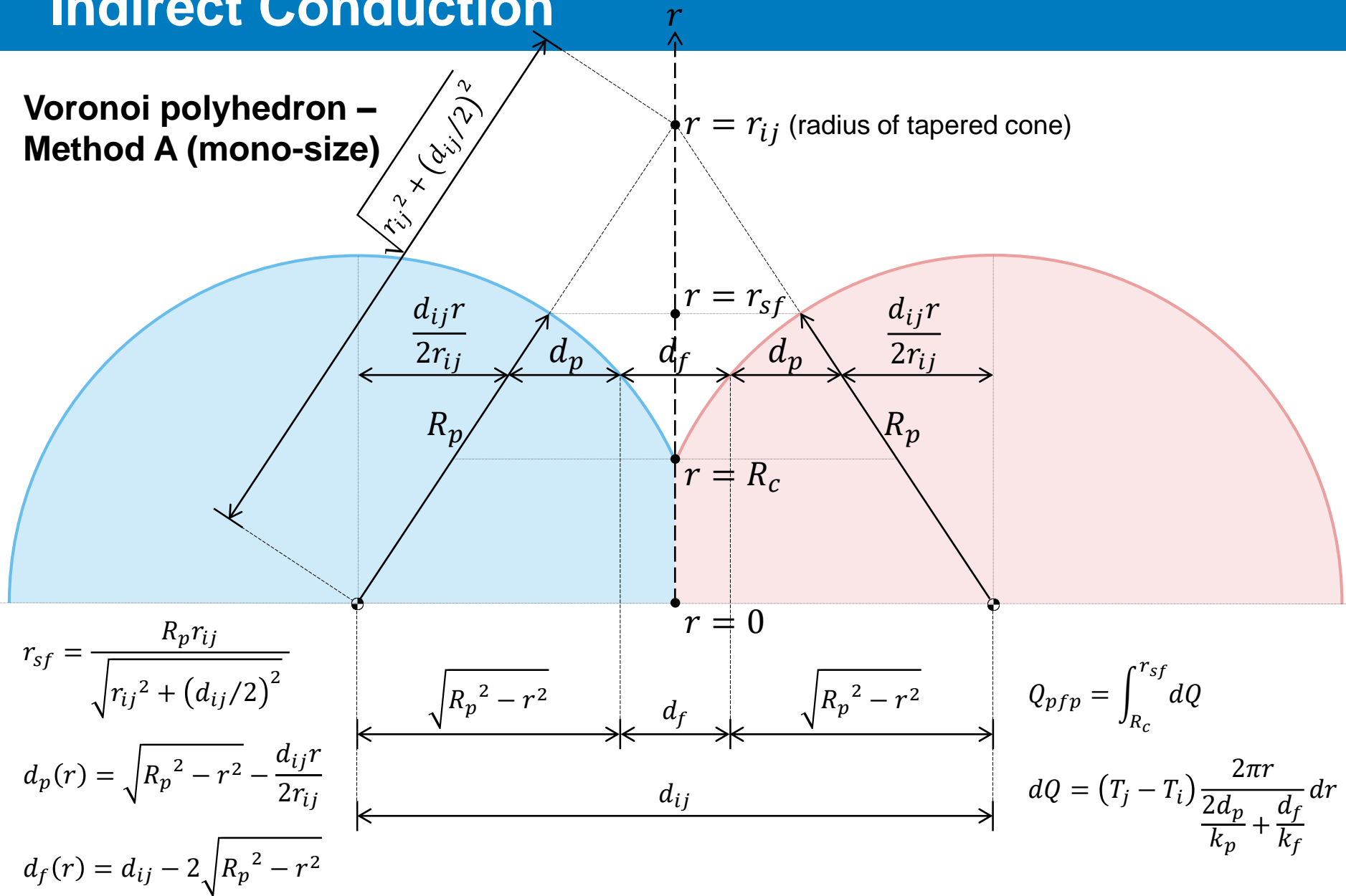
Voronoi polyhedron – Method A (interaction with walls)

Interaction with flat walls can be similarly addressed by adapting the geometry:

No suggestion on determining r_{ij} with walls has been found
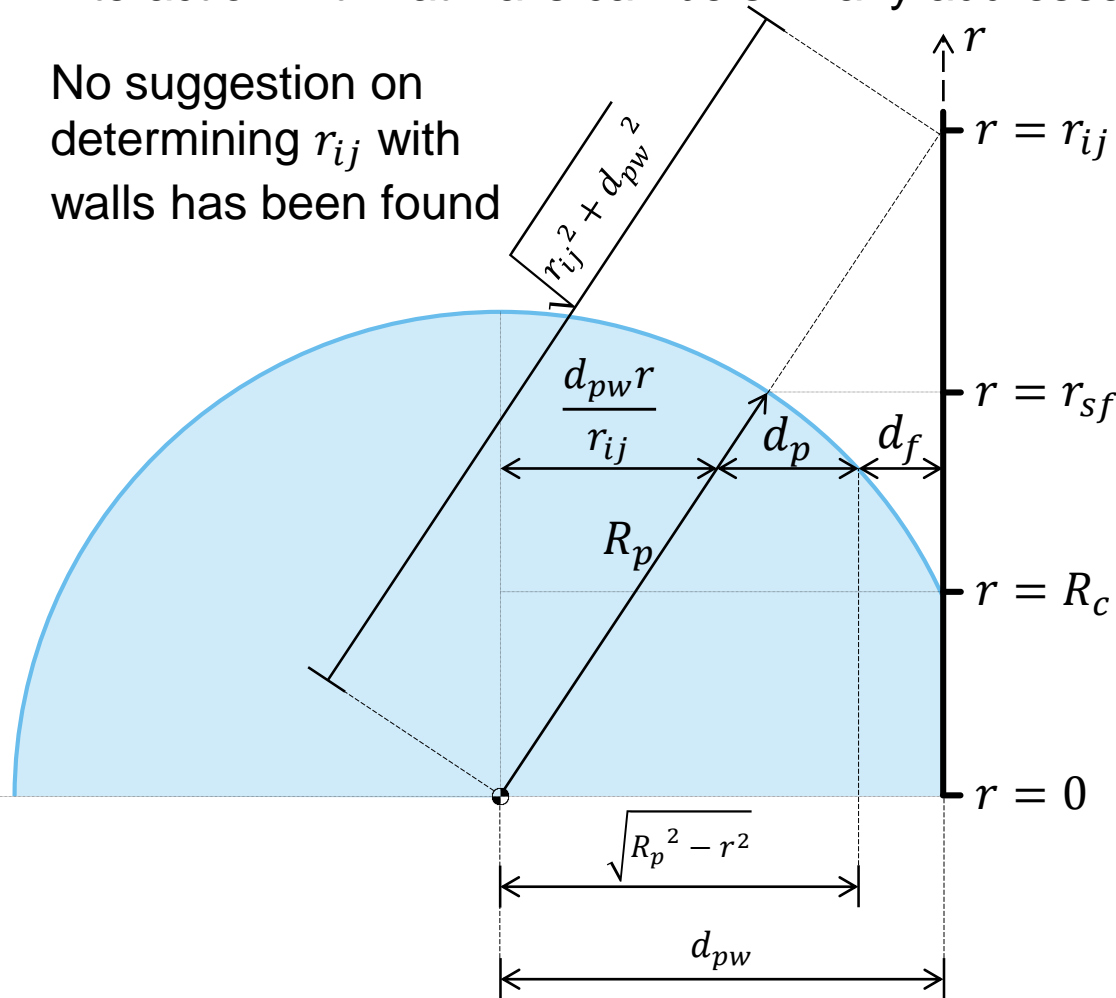
$$r_{sf} = \frac{R_p r_{ij}}{\sqrt{r_{ij}^2 + d_{pw}^2}}$$

$$d_p(r) = \sqrt{R_p^2 - r^2} - \frac{d_{pw} r}{r_{ij}}$$

$$d_f(r) = d_{pw} - \sqrt{R_p^2 - r^2}$$

The heat transfer rate is then:

$$Q_{pfw} = \int_{R_c}^{r_{sf}} dQ$$

$$dQ = (T_j - T_i) \frac{2\pi r}{\frac{d_p}{k_p} + \frac{d_f}{k_f}} dr$$

Conduction within the wall is not being considered.

Voronoi polyhedron – Method A (multiple-sizes)

For multi-sized particles, Norouzi et al (2016) suggested applying the same formula by simply using the average radius:

$$R_p = \frac{R_i + R_j}{2}$$

Gan et al (2016), on the other hand, extended this method for ellipsoids with different sizes (however, a validation for multi-sized spheres has not been reported).

$$Q_{pfp} = (T_j - T_i) \int_{R_c}^{r_{sf}} \frac{2\pi r}{\frac{1}{k_i}\left(\beta_i - \frac{D_i r}{r_{ij}}\right) + \frac{1}{k_j}\left(\beta_j - \frac{D_j r}{r_{ij}'}\right) + \left(\frac{d_{ij} - \beta_i - \beta_j}{k_f}\right)} dr$$

$$\beta_i = \sqrt{R_i{}^2 - r^2} \qquad \beta_j = \sqrt{R_j{}^2 - r^2}$$

When particles are not in contact, $R_c = 0$.

Indirect Conduction

Voronoi polyhedron – Method A (multiple-sizes)

$$D_i = \begin{cases} \dfrac{R_i^2 - R_j^2 + d_{ij}^2}{2d_{ij}} & \text{if} \quad \text{particles are not in contact} \\[2em] \sqrt{R_i^2 - R_c^2} & \text{if} \quad \text{particles are in contact} \end{cases}$$

$$D_j = d_{ij} - D_i$$

$$r_{sf} = \begin{cases} \dfrac{R_i r_{ij}}{\sqrt{r_{ij}^2 + D_i^2}} & \text{if} \quad R_i \leq R_j \\[2em] \dfrac{R_j r_{ij}}{\sqrt{r_{ij}^2 + D_j^2}} & \text{if} \quad R_i > R_j \end{cases}$$

Since r_{sf} is calculated based on the smaller particle, it might underestimate the heat transfer when particles have very different sizes (Peng et al, 2020).

$$r_{ij}' = \frac{D_j r_{sf}}{\sqrt{R_j^2 - r_{sf}^2}}$$

Voronoi polyhedron – Method B

- Each particle has an isothermal core of radius r_c, with the particle representative temperature.

- Heat transfer paths radiate from the cores' surfaces.

These assumptions lead to an expression that, although it does not need to solve an integral numerically, relies on an input fitting parameter (the radius of isothermal core).
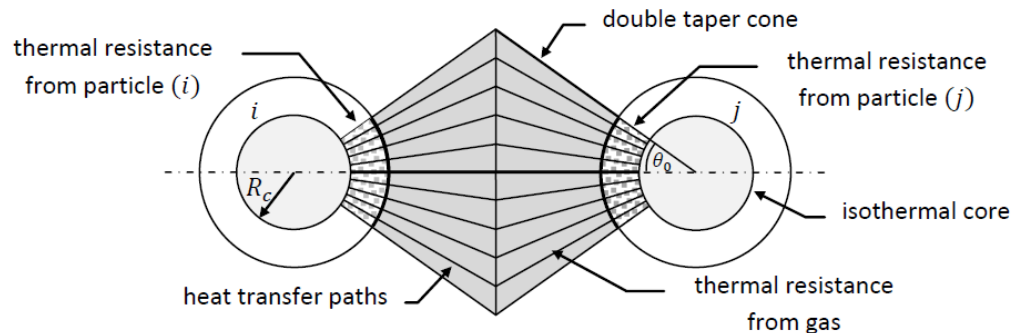
Figure 3-14: Cheng, Yu, and Zulli's [65] *Model B* for particle-fluid-particle conduction assumes that each particle has an isothermal core and the paths of heat transfer radiate from the particles centers.

Musser (2011)
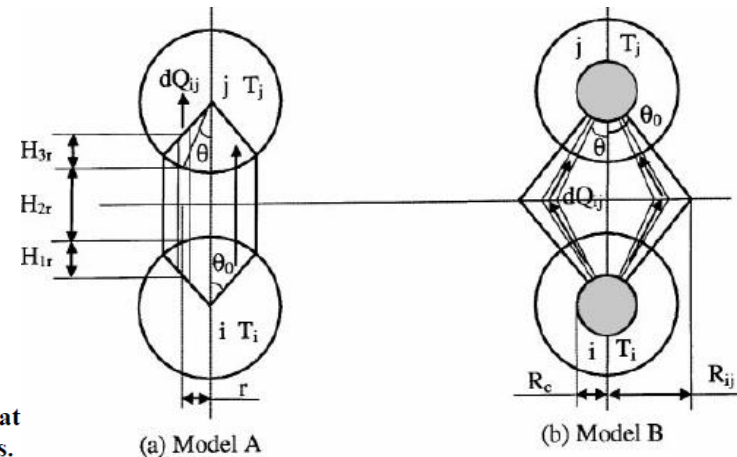
Cheng et al (1999)

Indirect Conduction

Voronoi polyhedron – Method B

The value of the isothermal core radius affects the results specially when k_p/k_f is not very high (< 1000), since a high ratio indicates that the resistance to heat conduction within particles is negligible.

For mono-sized particles, Cheng et al (1999) observed that $r_c = 0.5R_p$ provides results that are in good agreement with model A.

For multiple-sized particles, Chen et al (2019) compared the numerical results with experimental data and suggested:

$$r_c = 0.5R_p \quad \text{if} \quad 5 < k_p/k_f < 10^4$$
$$r_c = 0.6R_p \quad \text{if} \quad 1 < k_p/k_f < 5$$

For $k_p/k_f < 1$, the isothermal core assumption no longer holds and model B is not valid.
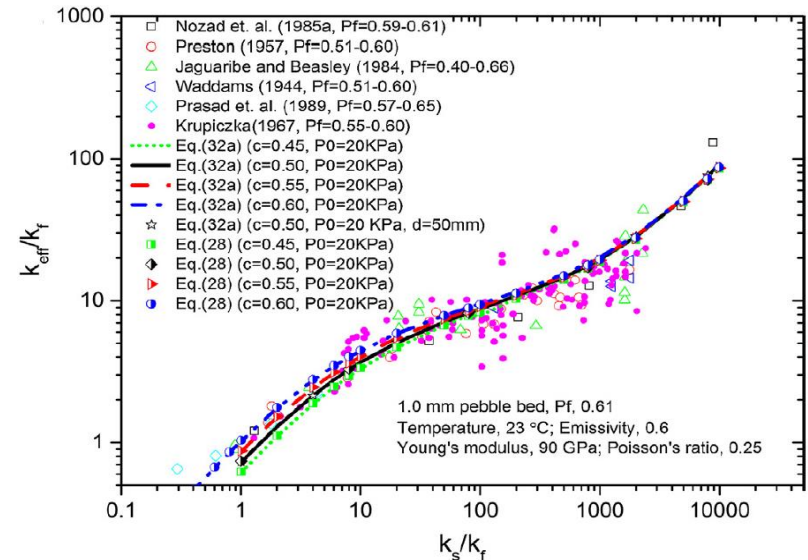
Chen et al (2019)

Indirect Conduction

Voronoi polyhedron – Method B (mono-size)

radial coordinates of each particle (for a given θ)

$(r_\theta, T_\theta), r_\theta = \dfrac{d_{ij}}{2\cos\theta}$

r_{ij} (radius of tapered cone)

$(R_p, T_{s,i})$ dQ_{fi} dQ_{fj} $(R_p, T_{s,j})$

dQ_i dQ_j

(r_c, T_i) R_c (r_c, T_j)

Particle i Particle j

θ_0 θ θ_c θ_c θ θ_0

d_{ij}

$\top r_i d\theta$ $r_j d\theta \top$

r_i $r_i \sin\theta$ $r_j \sin\theta$ r_j

θ θ

4 paths of heat flow from particle j to i:

1) Inside particle j (dQ_j):   from $r_j = r_c$ to $r_j = R_p$

2a) Through fluid (dQ_{fj}):   from $r_j = R_p$ to $r_j = r_\theta$

2b) Through fluid (dQ_{fi}):   from $r_i = r_\theta$ to $r_i = R_p$

3) Inside particle i (dQ_i):   from $r_i = R_p$ to $r_i = r_c$

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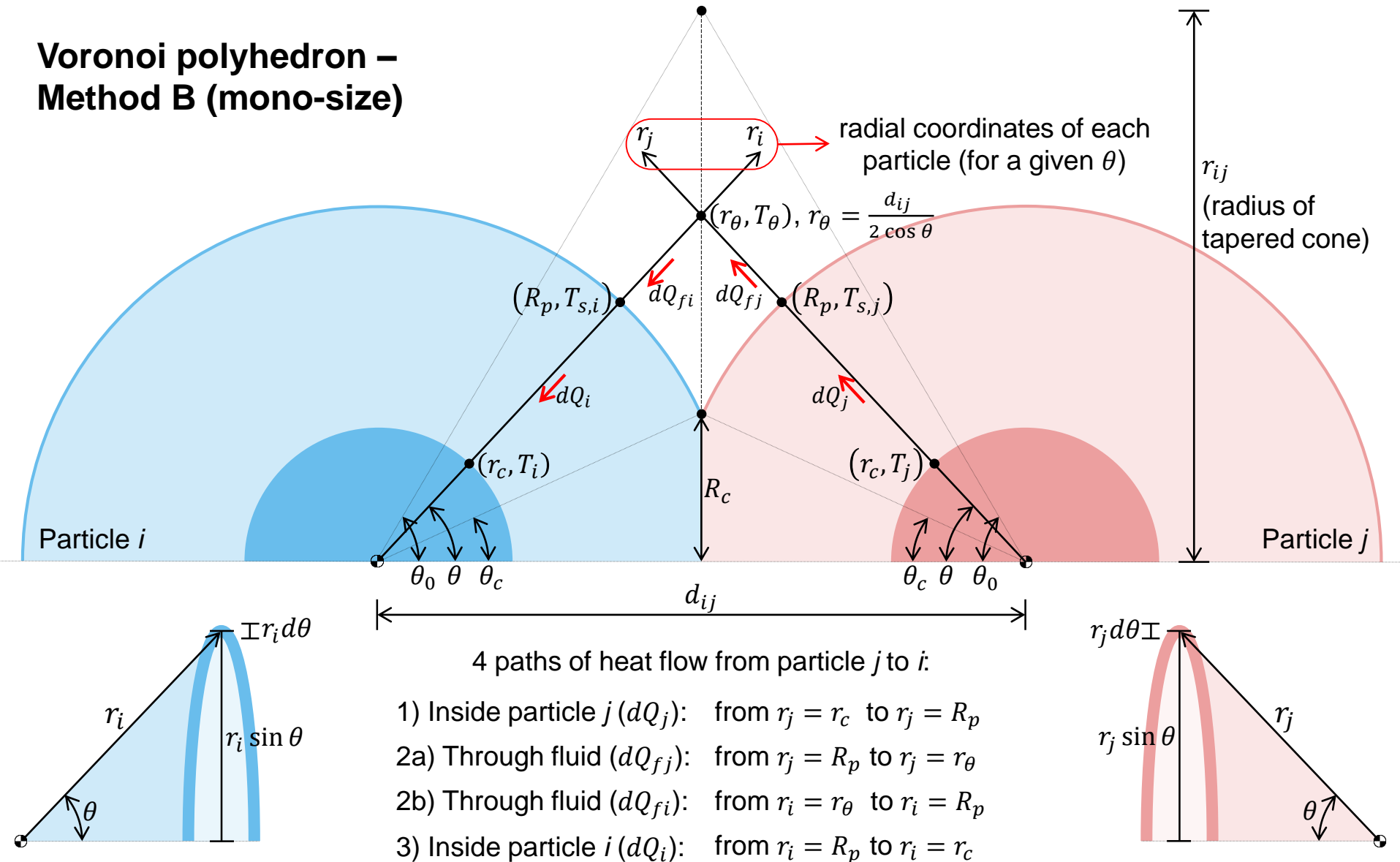
Indirect Conduction

Voronoi polyhedron – Method B (mono-size)

$$dQ_j = \left(r_j d\theta \cdot 2\pi r_j \sin\theta\right)\left(-k_j \, dT/dr_j\right) = -2\pi k_j r_j^2 \sin\theta \, d\theta \, dT/dr_j \quad \rightarrow \quad dT = -\frac{dQ_j}{2\pi k_j \sin\theta \, d\theta}\frac{dr_j}{r_j^2}$$

$$\left.\begin{array}{l} r_j = r_c \rightarrow T = T_j \\ r_j = R_p \rightarrow T = T_{s,j} \end{array}\right\} \qquad \int_{T_j}^{T_{s,j}} dT = \int_{r_c}^{R_p} -\frac{dQ_j}{2\pi k_j \sin\theta \, d\theta}\frac{dr_j}{r_j^2} \qquad \rightarrow \qquad \boxed{T_j - T_{s,j} = \frac{dQ_j}{2\pi k_j \sin\theta \, d\theta}\left(\frac{1}{r_c} - \frac{1}{R_p}\right)}$$

$$dQ_{fj} = \left(r_j d\theta \cdot 2\pi r_j \sin\theta\right)\left(-k_f \, dT/dr_j\right) = -2\pi k_f r_j^2 \sin\theta \, d\theta \, dT/dr_j \rightarrow \quad dT = -\frac{dQ_{fj}}{2\pi k_f \sin\theta \, d\theta}\frac{dr_j}{r_j^2}$$

$$\left.\begin{array}{l} r_j = R_p \rightarrow T = T_{s,j} \\ r_j = r_\theta \rightarrow T = T_\theta \end{array}\right\} \qquad \int_{T_{s,j}}^{T_\theta} dT = \int_{R_p}^{r_\theta} -\frac{dQ_{fj}}{2\pi k_f \sin\theta \, d\theta}\frac{dr_j}{r_j^2} \qquad \rightarrow \qquad \boxed{T_{s,j} - T_\theta = \frac{dQ_{fj}}{2\pi k_f \sin\theta \, d\theta}\left(\frac{1}{R_p} - \frac{1}{r_\theta}\right)}$$

$$dQ_{fi} = \left(r_i d\theta \cdot 2\pi r_i \sin\theta\right)\left(k_f \, dT/dr_i\right) = 2\pi k_f r_i^2 \sin\theta \, d\theta \, dT/dr_i \qquad \rightarrow \quad dT = \frac{dQ_{fi}}{2\pi k_f \sin\theta \, d\theta}\frac{dr_i}{r_i^2}$$

$$\left.\begin{array}{l} r_i = r_\theta \rightarrow T = T_\theta \\ r_i = R_p \rightarrow T = T_{s,i} \end{array}\right\} \qquad \int_{T_\theta}^{T_{s,i}} dT = \int_{r_\theta}^{R_p} \frac{dQ_{fi}}{2\pi k_f \sin\theta \, d\theta}\frac{dr_i}{r_i^2} \qquad \rightarrow \qquad \boxed{T_\theta - T_{s,i} = \frac{dQ_{fi}}{2\pi k_f \sin\theta \, d\theta}\left(\frac{1}{R_p} - \frac{1}{r_\theta}\right)}$$

$$dQ_i = \left(r_i d\theta \cdot 2\pi r_i \sin\theta\right)\left(k_i \, dT/dr_i\right) = 2\pi k_i r_i^2 \sin\theta \, d\theta \, dT/dr_i \qquad \rightarrow \quad dT = \frac{dQ_i}{2\pi k_i \sin\theta \, d\theta}\frac{dr_i}{r_i^2}$$

$$\left.\begin{array}{l} r_i = R_p \rightarrow T = T_{s,i} \\ r_i = r_c \rightarrow T = T_i \end{array}\right\} \qquad \int_{T_{s,i}}^{T_i} dT = \int_{R_p}^{r_c} \frac{dQ_i}{2\pi k_i \sin\theta \, d\theta}\frac{dr_i}{r_i^2} \qquad \rightarrow \qquad \boxed{T_{s,i} - T_i = \frac{dQ_i}{2\pi k_i \sin\theta \, d\theta}\left(\frac{1}{r_c} - \frac{1}{R_p}\right)}$$

Indirect Conduction

Voronoi polyhedron – Method B (mono-size)

Adding the resulting highlighted equations and rearranging the terms (the terms $dQ_i = dQ_j = dQ_{fi} = dQ_{fj}$ are expressed simply as dQ):

$$dQ = \frac{T_j - T_i}{\dfrac{1/r_c - 1/R_p}{2\pi k_i \sin\theta} + \dfrac{1/r_c - 1/R_p}{2\pi k_j \sin\theta} + \dfrac{1/R_p - 1/r_\theta}{\pi k_f \sin\theta}}\, d\theta = \left(T_j - T_i\right)\pi \frac{\sin\theta}{a - b\cos\theta}\, d\theta$$

Where:
$$a = \frac{1}{2\bar{k}}\left(\frac{1}{r_c} - \frac{1}{R_p}\right) + \frac{1}{k_f R_p} \qquad b = \frac{2}{k_f d_{ij}}$$

The total heat transfer rate is obtained by integrating the elementary heat rate over the range of angles that define the tapered cone:

$$Q_{pfp} = \int_{\theta_c}^{\theta_0} dQ = \left(T_j - T_i\right)\pi \int_{\theta_c}^{\theta_0} \frac{\sin\theta}{a - b\cos\theta}\, d\theta$$

Voronoi polyhedron – Method B (mono-size)

Cheng et al (1999) performed this integration and determined that the particle-fluid-particle heat transfer rate by conduction can be expressed as:

$$Q_{pfp} = \left(T_j - T_i\right) \frac{\pi}{b} \ln\left(\frac{a - b \cos \theta_0}{a - b \cos \theta_c}\right)$$

$$a = \frac{1}{2\bar{k}}\left(\frac{1}{r_c} - \frac{1}{R_p}\right) + \frac{1}{k_f R_p}$$

$$\cos \theta_0 = \frac{d_{ij}}{2\sqrt{r_{ij}^2 + \left(d_{ij}/2\right)^2}}$$

$$b = \frac{2}{k_f d_{ij}}$$

$$\cos \theta_c = \frac{d_{ij}}{2\sqrt{R_c^2 + \left(d_{ij}/2\right)^2}}$$

When particles are not in contact, $R_c = 0$.

Indirect Conduction

Voronoi polyhedron – Method B (interaction with walls)

Interaction with flat walls can be similarly addressed by adapting the geometry:

No suggestion on determining r_{ij} with walls has been found
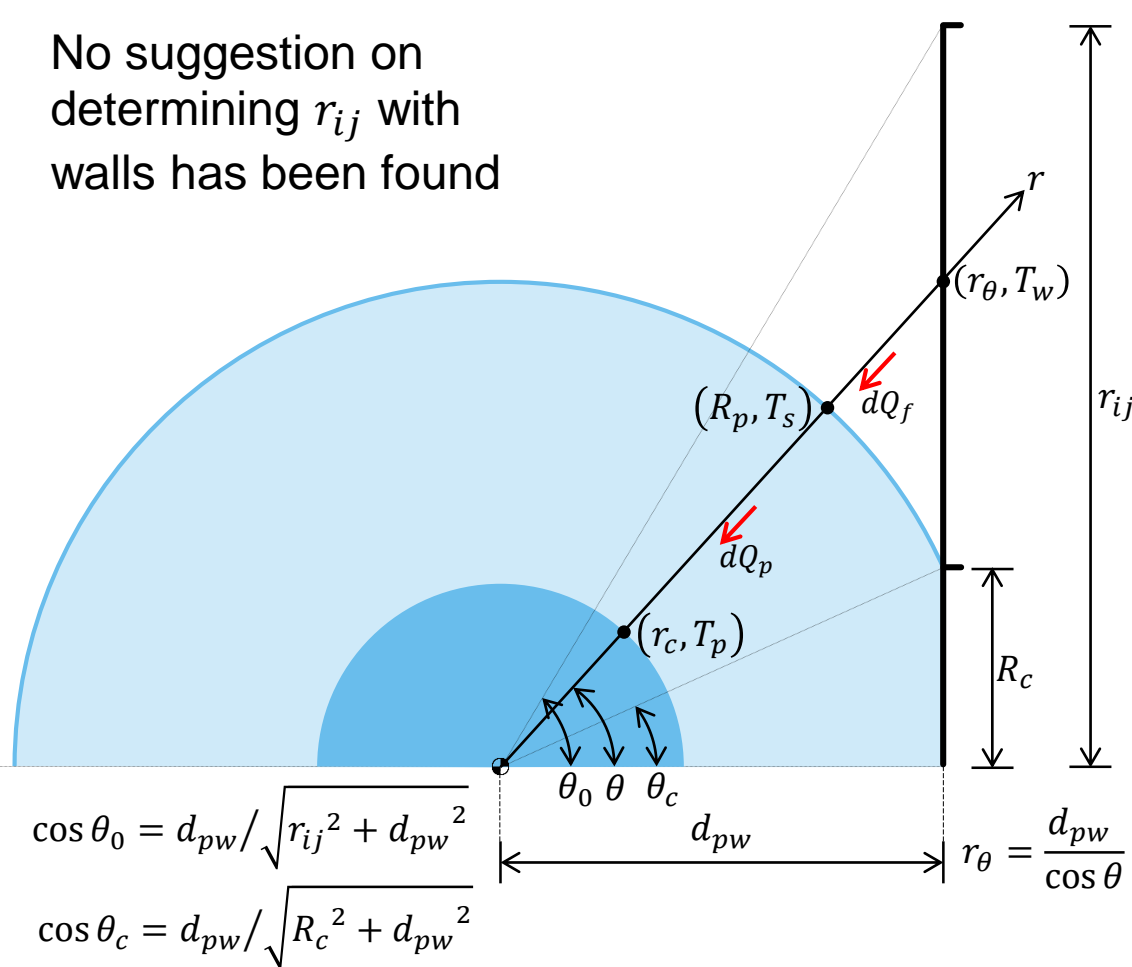
$$dQ_f = 2\pi k_f r^2 \sin\theta \, d\theta \, dT/dr$$
$$dQ_p = 2\pi k_p r^2 \sin\theta \, d\theta \, dT/dr$$

$$T_w - T_s = \frac{dQ_f}{2\pi k_f \sin\theta \, d\theta}\left(\frac{1}{R_p} - \frac{1}{r_\theta}\right)$$

$$T_s - T_p = \frac{dQ_p}{2\pi k_p \sin\theta \, d\theta}\left(\frac{1}{r_c} - \frac{1}{R_p}\right)$$

$$dQ = \frac{T_w - T_p}{\dfrac{1/r_c - 1/R_p}{2\pi k_p \sin\theta} + \dfrac{1/R_p - 1/r_\theta}{2\pi k_f \sin\theta}} d\theta$$

$$Q_{pfw} = (T_w - T_p)\frac{\pi}{b}\ln\left(\frac{a - b\cos\theta_0}{a - b\cos\theta_c}\right)$$

$$\cos\theta_0 = d_{pw}/\sqrt{r_{ij}^2 + d_{pw}^2}$$
$$\cos\theta_c = d_{pw}/\sqrt{R_c^2 + d_{pw}^2}$$

$$r_\theta = \frac{d_{pw}}{\cos\theta}$$

$$a = \frac{1}{2k_p}\left(\frac{1}{r_c} - \frac{1}{R_p}\right) + \frac{1}{2k_f R_p} \qquad b = \frac{1}{2k_f d_{pw}}$$

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Voronoi polyhedron – Method B (multiple-sizes)

For multi-sized particles, Chen et al (2019) improved the method:

$$\Lambda > 0 \quad \rightarrow \quad Q_{pfp} = \left(T_j - T_i\right)\frac{\pi k_f d_{ij}(1 - \Delta\gamma^2)}{2\sqrt{|\Lambda|}}\ln\left|\frac{1 - Y_1}{1 + Y_1}\right|$$

$$\Lambda = 0 \quad \rightarrow \quad Q_{pfp} = \left(T_j - T_i\right)\frac{\pi k_f d_{ij}(1 - \Delta\gamma^2)}{A + B}\left(\frac{1}{\delta_i^{\min}} - \frac{1}{\delta_i^{\max}}\right)$$

$$\Lambda < 0 \quad \rightarrow \quad Q_{pfp} = \left(T_j - T_i\right)\frac{\pi k_f d_{ij}(1 - \Delta\gamma^2)}{2\sqrt{|\Lambda|}}\tan^{-1}(Y_2)$$

where:
$$\begin{cases} \Lambda = (1 + \Delta\gamma A)(1 - \Delta\gamma B) \\[2mm] \Delta\gamma = \gamma_j - \gamma_i \quad \begin{cases} \gamma_i = R_i/d_{ij} \\ \gamma_j = R_j/d_{ij} \end{cases} \end{cases}$$

For mono-sized particles $\gamma_i = \gamma_j$, and this model reduces to the original one of Cheng et al (1999).

Voronoi polyhedron – Method B (multiple-sizes)

$$Y_1 = \frac{X_{\max} - X_{\min}}{1 - X_{\max}X_{\min}}$$

$$Y_2 = \frac{X_{\max} - X_{\min}}{1 + X_{\max}X_{\min}}$$

$$X_{\max} = \frac{(A + B)\delta_i^{\max} + \Delta\gamma B - 1}{\sqrt{|\Lambda|}}$$

$$X_{\min} = \frac{(A + B)\delta_i^{\min} + \Delta\gamma B - 1}{\sqrt{|\Lambda|}}$$

$$A = \frac{k_i + k_f(R_i/r_{c,i} - 1)}{k_i\gamma_i}$$

$$B = \frac{k_j + k_f(R_j/r_{c,j} - 1)}{k_j\gamma_j}$$

$$\delta_i^{\max} = \frac{1}{2}\left(\sqrt{1 + \frac{4A_n}{\pi d_{ij}^2(1 - \Delta\gamma^2)}} - \Delta\gamma\right)$$

$$\delta_i^{\min} = \frac{1}{2}\left(\sqrt{1 + \frac{4R_c^2}{d_{ij}^2(1 - \Delta\gamma^2)}} - \Delta\gamma\right)$$

A_n is the nominal area for the neighboring Voronoi cells.

When particles are not in contact, $R_c = 0$.

Indirect Conduction

Voronoi polyhedron methods – Remarks

When particles are moving, it is computationally demanding to build the transient Voronoi polyhedra at every time step.

However, the only parameters of the previous methods that depend on the shape of the polyhedra are the volume V_{ij}, to compute the radius r_{ij}, and the area A_n.

Yang et al (2002) stablished a relationship between the average face area of the Voronoi polyhedra and the packing density of mono-sized fine particles.

Zhou et al (2009) used these results to compute the mentioned parameters from the local porosity ε_i (i.e. local void fraction) around particle *i*, which is usually an output of DEM simulations so that the Voronoi tessellation would not be needed:

$$A_n = 0.985 R_i^{\,2} (1 - \varepsilon_i)^{-2/3} \qquad\qquad r_{ij} = \sqrt{A_n/\pi} = 0.560 R_i (1 - \varepsilon_i)^{-1/3}$$

P.S. For multi-sized particles, the radius of particle *i*, R_i, is used to compute r_{ij}.

Indirect Conduction

Voronoi polyhedron methods – Remarks

The particle-fluid-particle conductive heat transfer rate decreases sharply when the distance between two non-contacting particles becomes larger.

When two particles are far away from each other, although their Voronoi polyhedra are neighbors, indirect conduction should be neglected.

Using method A with mono-sized spheres, Zhou et al (2009) suggested that indirect conduction can be ignored when the distance between the surfaces of two particles is greater than or equal to their radius ($d_{ij} \geq 3R_p$).

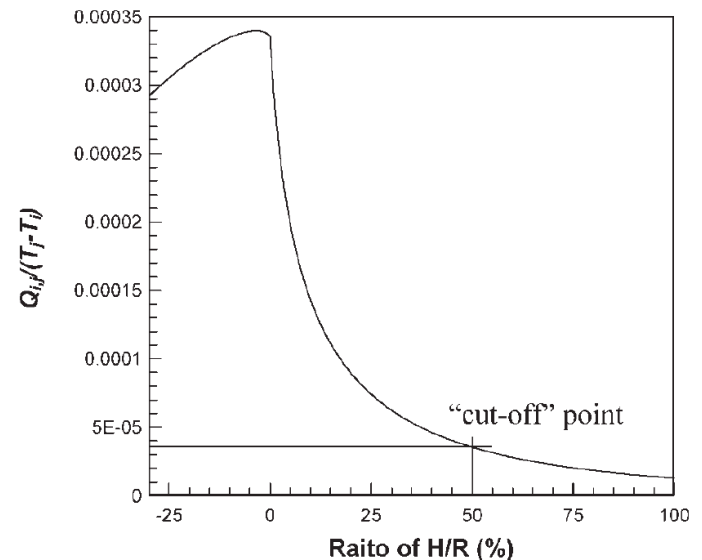For the other models, a similar cut-off value should be set.

Figure 2. Variation of $Q_{i,j}/(T_j - T_i)$ with the ratio of H/R (%), calculated by Eq. 14a.

Zhou et al (2009)

Indirect Conduction

Surrounding layer method

Introduced by Rong & Horio (1999), similarly to Delvosalle and Vanderschuren (1985), for mono-sized particles and later modified by Musser (2011) for multi-sized particles.

- Each particle is surrounded by a fluid layer of thickness δ_f, proportional to its radius.

- Heat transfer starts when the layer of a particle intersects the surface of another (i.e. $d_{ij} < R_i + R_j + \max(\delta_{f,i}, \delta_{f,j})$).

- A thin uniform fluid layer separates the particles' surfaces when they are in contact (i.e. there is a minimum separation, or conduction, distance of thickness S).

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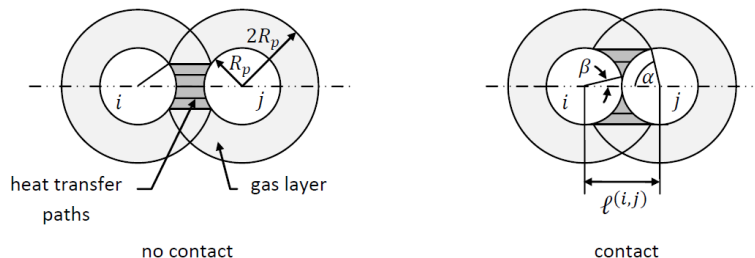
Figure 3-15: Rong and Horio's [16] configuration for particle-fluid-particle conduction. In their model, each particle is surrounded by a gas layer and heat transfer occurs across paths parallel to the line connecting the centers of the particles. When particles engage in contact, the overlap region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

Musser (2011)
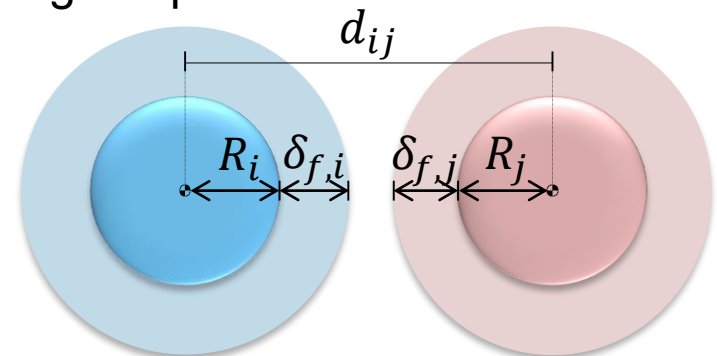
The fluid layer considered as "static" due to no-slip condition over small distances and no density-driven flow (Lattanzi & Hrenya, 2017)

Indirect Conduction

Surrounding layer – Method by Rong & Horio (1999)

For mono-sized particles of radius R_p, the heat conduction is calculated as:

$$2R_p + \delta_f > d_{ij} > 2R_p$$

(fluid layers Intersecting surfaces)

$$\rightarrow \quad Q_{pfp} = (T_j - T_i)k_f \int_0^{\theta_2} \frac{2\pi R_p \sin\theta}{d_{ij} - 2R_p \cos\theta} d(R_p \sin\theta)$$

Heat fluxes over the non-contacting region

$$d_{ij} \leq 2R_p$$

(Particles in contact)

$$\rightarrow \quad Q_{pfp} = (T_j - T_i)k_f \int_{\theta_1}^{\theta_2} \frac{2\pi R_p \sin\theta}{d_{ij} - 2R_p \cos\theta} d(R_p \sin\theta)$$

$$+(T_j - T_i)k_f \frac{\pi(R_p \sin\theta_1)^2}{S}$$

Uniform conduction across the contact area, through the minimum separation distance (it was considered as the Q_{cpp})

Where:

$$\theta_1 = \max\left(\cos^{-1}\left(\frac{d_{ij}}{2R_p}\right), \cos^{-1}\left(\frac{2R_p - S}{2R_p}\right)\right)$$

$$\theta_2 = \cos^{-1}\left(\frac{d_{ij}^2 + R_p^2 - (R_p + \delta_f)^2}{2R_p d_{ij}}\right)$$

Indirect Conduction

Surrounding layer – Method by Musser (2011)

- Discarded the contact conduction term, since it is already being considered by the appropriate methods presented previously for direct heat conduction.

- Modified the geometry to consider multi-sized particles.

- Changed variables to allow the integral to be solved by basic quadrature routines.

$$Q_{pfp} = (T_j - T_i)k_f \int_{R_c}^{R_f} \frac{2\pi r}{\max\left(S, d_{ij} - \sqrt{R_i^2 - r^2} - \sqrt{R_j^2 - r^2}\right)} dr$$

Where:

$$R_f = \sqrt{\left(R_k + \delta_{f,k}\right)^2 - \left(\left(\left(R_k + \delta_{f,k}\right)^2 - R_l^2 + d_{ij}^2\right)/2d_{ij}\right)^2} \qquad \begin{cases} R_k = \max(R_i, R_j) \\ R_l = \min(R_i, R_j) \end{cases}$$

$$R_c = \begin{cases} 0 & \text{if} \quad d_{ij} > R_i + R_j \quad \text{(i.e. particles are not in contact)} \\ R_c^{geo} & \text{if} \quad d_{ij} \leq R_i + R_j \quad \text{(i.e. particles are in contact)} \end{cases}$$

Indirect Conduction

$\delta_{f,i}$

r

$d_f(r)$

R_i

R_f

R_f

R_j

R_c

$\delta_{f,j}$

$\sqrt{R_i^2 - R_f^2}$

$d_f(R_f)$

$\sqrt{R_j^2 - R_f^2}$

$\sqrt{R_i^2 - R_c^2}$

$d_f(R_c) = 0$

$\sqrt{R_j^2 - R_c^2}$

d_{ij}

$d_f(r)$ is the conduction distance through the fluid layer (denominator of the integrand)

$$d_f(r) = d_{ij} - \sqrt{R_i^2 - r^2} - \sqrt{R_j^2 - r^2}$$

Since $d_f(r = R_c) = 0$, there is a singularity at this point, so the value of S is assumed when $d_f(r) < S$
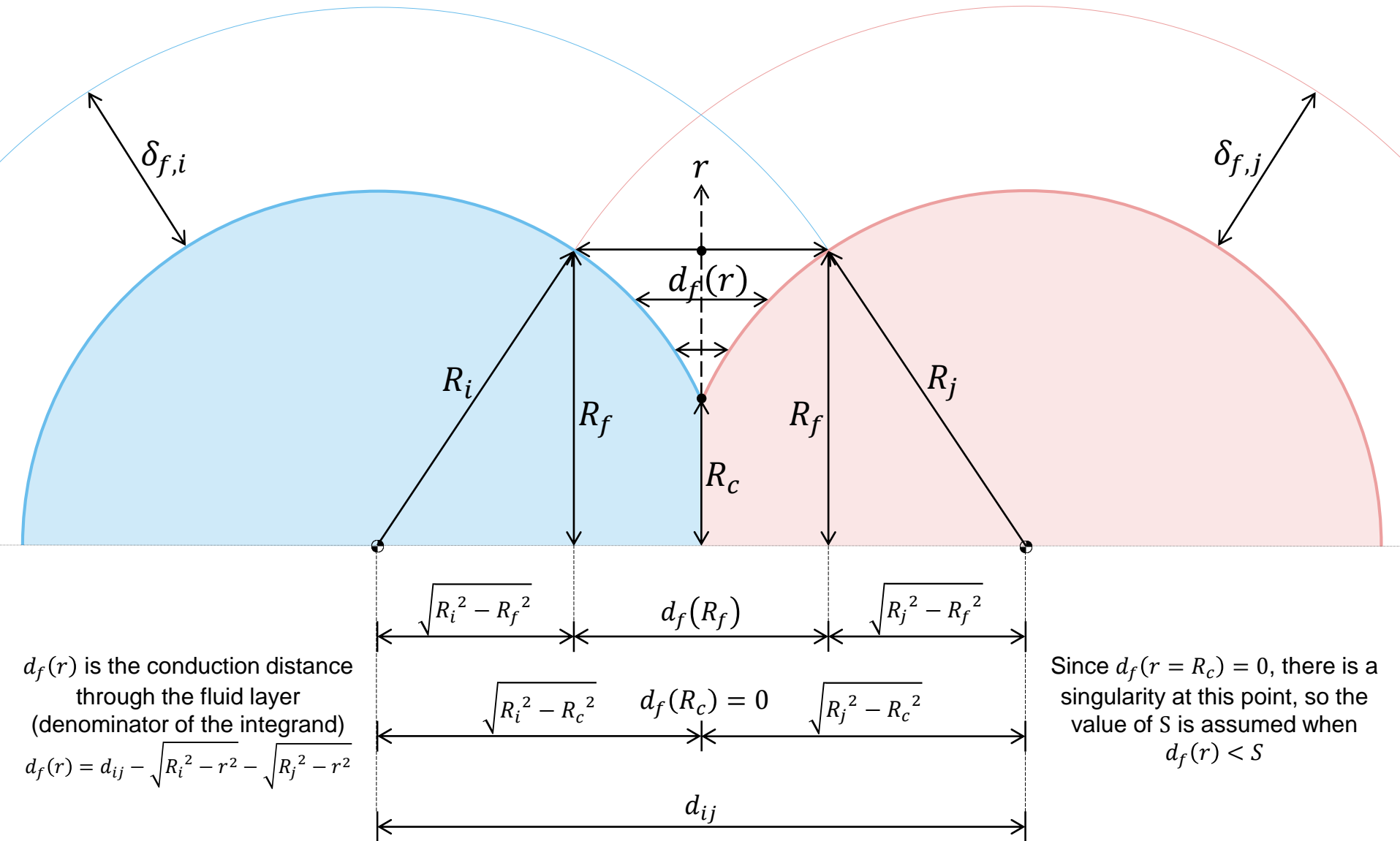
Indirect Conduction

Surrounding layer method – Lower boundary
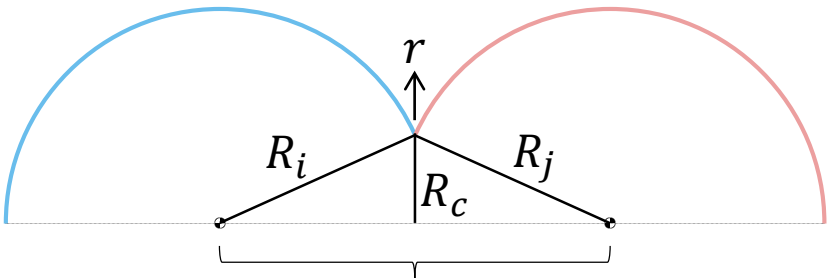
At the lower boundary R_c, the denominator becomes zero (i.e. an infinite heat flow) if the value of S is not considered as a minimum threshold value.

Mathematically, the minimum separation is needed to avoid a singularity in the integral term when particles are touching.

Physically, the minimum separation is related to the height of the surface asperities, so its value is sometimes determined by the surface roughness in non-smooth particles.

By applying the minimum separation when the denominator goes to zero, the issue is corrected by prohibiting a perfect contact between particles.

Due to the sharp variations across the integral boundary, a robust quadrature should be used for integrating (Musser, 2011, suggested an Adaptive Simpson's method).

$$d_{ij} = \sqrt{R_i^2 - R_c^2} + \sqrt{R_j^2 - R_c^2}$$

This condition nullifies the denominator!

Indirect Conduction

Surrounding layer method – Upper boundary

The upper boundary R_f, must be limited to the size of the radius of the smaller particle:

This is applicable when the fluid layer of one sphere intersects the surface of the other sphere in a point beyond its centerline perpendicular to the flow paths.
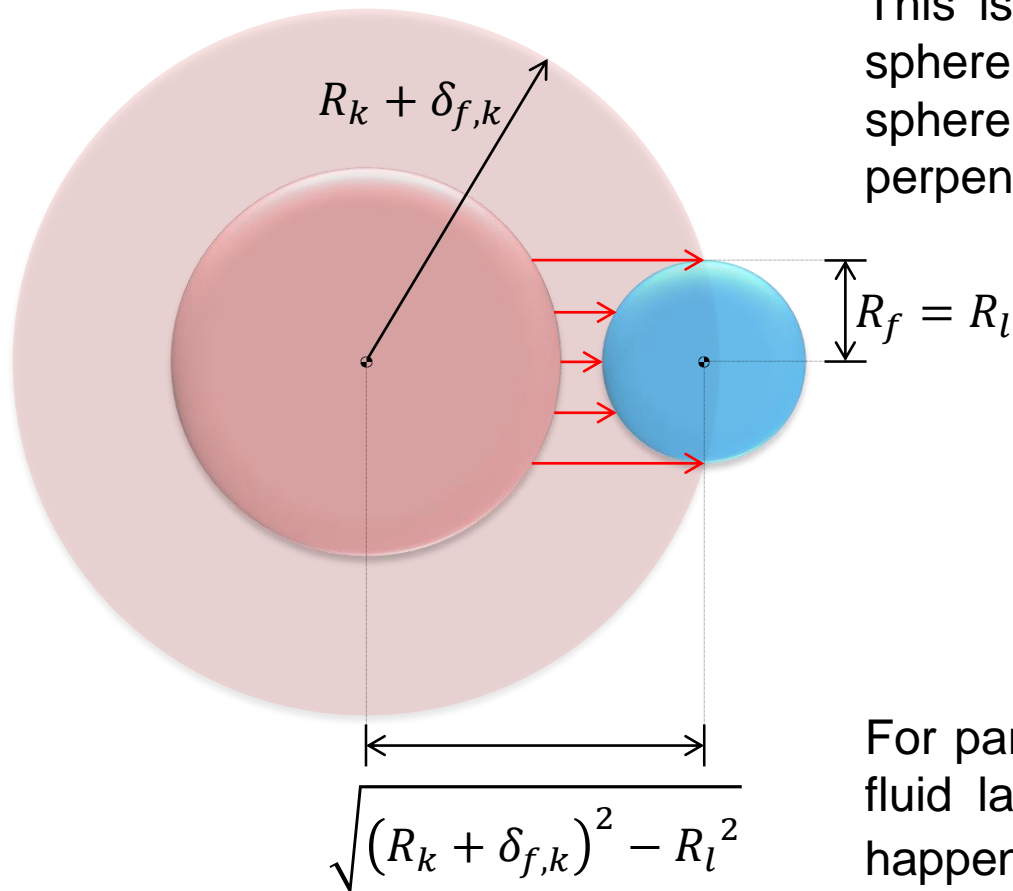
$R_f = R_l$

If $d_{ij} \leq \sqrt{\left(R_k + \delta_{f,k}\right)^2 - R_l^2}$

then $R_f = R_l$

where: $\begin{cases} R_k = \max(R_i, R_j) \\ R_l = \min(R_i, R_j) \end{cases}$

For particles with the same size, the maximum fluid layer thickness to avoid this situation to happen is $\delta_f = \left(\sqrt{2} - 1\right)R_p \cong 0.41R_p$

$R_k + \delta_{f,k}$

$\sqrt{\left(R_k + \delta_{f,k}\right)^2 - R_l^2}$

Surrounding layer method – Interaction with walls

Interaction with flat walls can be similarly addressed by adapting the geometry:
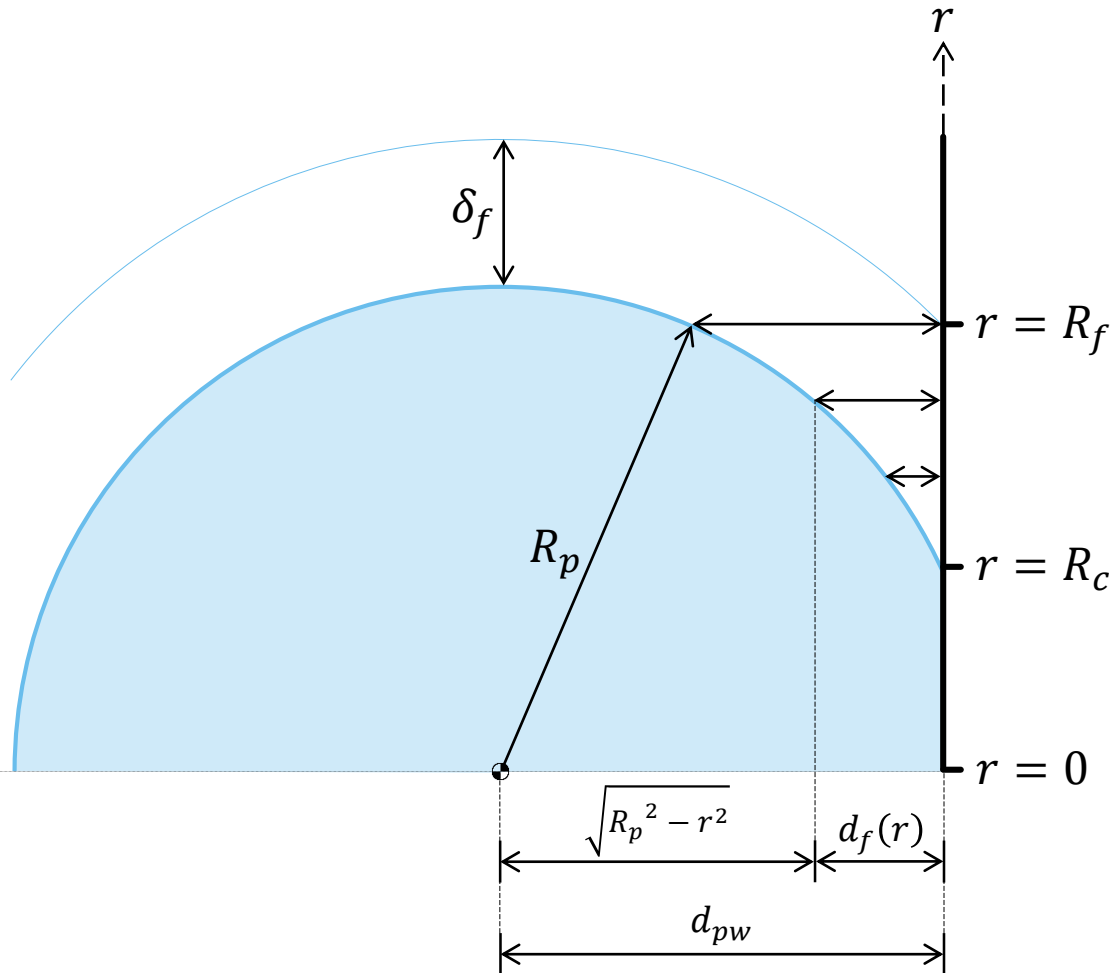
$$Q_{pfw} = (T_w - T_p)k_f \int_{R_c}^{R_f} \frac{2\pi r}{\max\left(S, d_f(r)\right)} dr$$

$$d_f(r) = d_{pw} - \sqrt{R_p^2 - r^2}$$

$$R_f = \sqrt{(R_p + \delta_f)^2 - d_{pw}^2}$$

The upper boundary, must be limited to the radius of the particle:

If $d_{pw} \leq \sqrt{(R_p + \delta_f)^2 - R_p^2}$

then $R_f = R_p$

Surrounding layer method – Contact with walls

For particle-wall contacts, an analytical solution for the integral expression was given in Morris (2015), Lattanzi & Hrenya (2017) and Lu et al (2017). One way to write it is:

$$Q_{pfw} = 2\pi(T_w - T_p)k_f R_p\big((a + 1)\ln(|b - a - 1|/|a - c + 1|) + b - c\big)$$

Where:

$$a = (d_{pw} - R_p)/R_p \qquad b = \sqrt{1 - r_{\text{out}}{}^2} \qquad c = \sqrt{1 - r_{\text{in}}{}^2}$$

$$r_{\text{in}} = \begin{cases} 0 & \text{if} \quad d_{pw} > R_p + S \\[2ex] \sqrt{1 - \left(\dfrac{S}{R_p} - a - 1\right)^2} & \text{if} \quad d_{pw} \leq R_p + S \end{cases}$$

$$r_{\text{out}} = \begin{cases} \sqrt{\left(\dfrac{R_p + \delta_f}{R_p}\right)^2 - (a + 1)^2} & \text{if} \quad a > \sqrt{\left((R_p + \delta_f)/R_p\right)^2 - 1} - 1 \\[3ex] 1 & \text{if} \quad a \leq \sqrt{\left((R_p + \delta_f)/R_p\right)^2 - 1} - 1 \end{cases}$$

Surrounding layer method – Input parameters

The method requires input values of two parameters for the particles:
fluid layer thickness δ_f, and minimum separation distance S.

Values of δ and s used for calculating the indirect particle-fluid-particle conduction by the surrounding layer method. (Peng et al, 2020)

Author(s)	Particle size d_p (mm)	Layer thickness δ(mm)	Min. conduction distance s (m)
Rong and Horio (1999)	1	r_p	4×10^{-10}
Morris et al. (2015)	0.3	$0.4r_p$	$2.75 \times 10^{-8} (\sim \lambda_g)$
Morris et al. (2016b)	0.3	$0.4r_p$	$2.75 \times 10^{-8} (\sim \lambda_g)$
Lattanzi and Hrenya (2016)	0.2	$0.4r_p$	$2.75 \times 10^{-8} (\sim \lambda_g)$
Lu et al. (2017)	1	$1.08r_p$	1×10^{-6}
Wang et al. (2019)	1	$0.2r_p$	Not given

In static or packed systems, the value of S has a more significant impact on the total amount of heat transfer compared to δ_f, and a large value is not recommended for static or dense particulate systems (Morris et al, 2015).

In dynamic or dilute systems, the results show strong dependence on the selected value of δ_f, but not on S (Lattanzi & Hrenya, 2017).

Although due attention must be given to these parameters, there is no guideline for selecting their values, so different justifications for the choice are found in the literature.

Indirect Conduction

Other methods – Vargas & McCarthy (2002)

Considers stagnant interstitial fluids (liquid + gas) in packed beds, separating the heat conduction through the liquid and gas phases between contacting particles only.

Applicable for low Reynolds number ($R_e \ll 1$), high particle conductivities ($k_p/k_f \gg 1$) and identical particles.

Depends on physical-chemical properties of particles obtained from the literature.

Investigated the dependency of the results with gas pressure, external load and saturation level: good agreement with experiments, when the assumptions are valid.

Assumes unidirectional heat flow and a liquid bridge between contacting particles, with a fixed filling angle φ for all contacts.

$$Q_{pfp} = \left(\frac{k_l A_l}{l_l} + \frac{k_g^* A_g}{l_g} \right) (T_j - T_i)$$

R_c is compute from Hertz theory for static loading
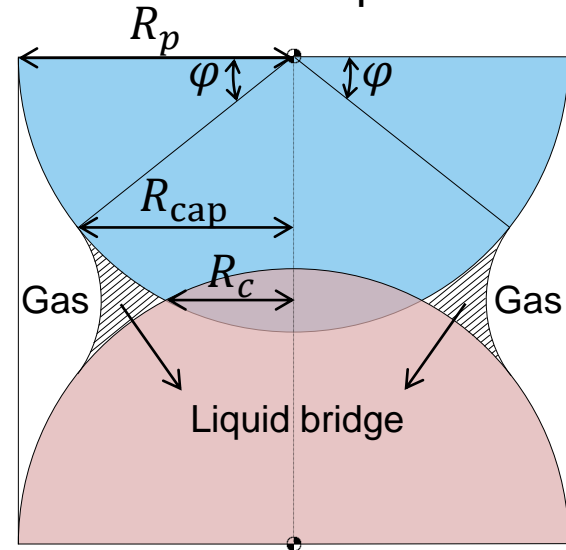
Other methods – Vargas & McCarthy (2002)

Surface areas exposed to liquid and gas:

$$A_c = \pi R_c{}^2$$

$$A_l = 4\pi R_p{}^2 \left(\left({}^{\pi}\!/_2 - \varphi \right) \tan \varphi - 1 + \cos \varphi \right) \left(\frac{1 - \cos \varphi}{\cos \varphi} \right) - A_c$$

$$A_g = 2\pi R_p{}^2 - A_l - A_C$$

Characteristic average lengths of over which the fluxes apply:

$$l_l = \frac{R_{\text{cap}} R_p - {}^1\!/_2 \left(\varphi R_p{}^2 + R_{\text{cap}} \sqrt{R_p{}^2 - R_{\text{cap}}{}^2} \right)}{R_{\text{cap}} - R_c}$$

$$l_g = \frac{R_p{}^2 \left(1 - {}^{\pi}\!/_4 \right)}{R_p - R_c} - l_l$$

$$R_{\text{cap}} = \sqrt{R_c{}^2 (1 - \cos \varphi)(1 + \cos \varphi)}$$

Indirect Conduction

Other methods – Vargas & McCarthy (2002)

Modified conductivity of gas phase appropriate to use over finite lengths:

$$k_g^* = k_g/(1 + M/l_g)$$

Where:

$$M = \left(\frac{2 - ac_i}{ac_i} + \frac{2 - ac_j}{ac_j}\right)\frac{\zeta}{\zeta + 1}\frac{1}{P_r}\omega$$

$$P_r = \frac{c_g\mu_g}{k_g} \text{ (Prandtl number)}$$

$$\omega = \frac{k_B T}{\sqrt{2}\pi d_g^2 P_g}$$

$\zeta \rightarrow$ Ratio of specific heats

$ac_i \rightarrow$ Thermal accommodation coefficient at particle surface: empirical parameter obtained from literature data

$P_g \rightarrow$ Gas pressure

$d_g \rightarrow$ Gas molecule diameter

$k_B \rightarrow$ Boltzman constant (1.3806×10^{-23})

$\omega \rightarrow$ Molecular mean free-path of gas

Molecule collision regime: The mean free-path is small w.r.t. mean separation distance ($k_g^* = k_g$).

Free molecule conduction regime: The mean free-path is large w.r.t. mean separation distance ($k_g^* \sim P_g$).

(up to atm pressure, this regime was observed in some gases, e.g. Helium, so the results vary with the interstitial gas pressure)

Other methods – Vargas & McCarthy (2002)

Interstitial fluid with only gas: $\varphi = A_l = l_l = 0$

$$\left.\begin{array}{l} A_g = 2\pi R_p{}^2 - \pi R_c{}^2 \\[2ex] l_g = \dfrac{R_p{}^2\left(1 - {}^\pi/_4\right)}{R_p - R_c} \end{array}\right\} \quad Q_{pfp} = k_g^*(T_j - T_i)\dfrac{2\pi\left(1 - {}^1/_2\left(R_c/R_p\right)^2\left(R_p - R_c\right)\right)}{1 - {}^\pi/_4}$$

Interstitial fluid with only liquid: $\varphi = \pi/2$ (as a limit)

$$\left.\begin{array}{l} A_l = 4\pi R_p{}^2 - \pi R_c{}^2 \\[2ex] l_l = \dfrac{R_p{}^2\left(1 - {}^\pi/_4\right)}{R_p - R_c} \end{array}\right\} \quad Q_{pfp} = k_l(T_j - T_i)\dfrac{4\pi\left(1 - {}^1/_2\left(R_c/R_p\right)^2\left(R_p - R_c\right)\right)}{1 - {}^\pi/_4}$$

3 – Convective Heat Transfer

Convective Heat Transfer

Thermal convection

Related to fluid motion: heat is carried along with the flow.
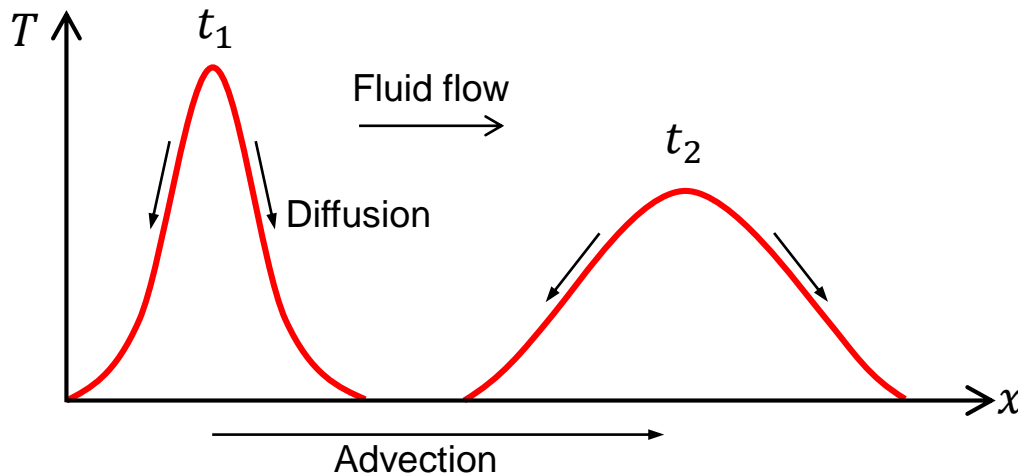
→**Natural convection**: Fluid motion caused by density change.

→**Forced convection**: Fluid motion forced by external agents.

The fluid motion induces heat transfer by:

→**Advection**: Heat transfer by the bulk motion of the fluid.

→**Diffusion**: Heat transfer by the collision of molecules due to temperature gradient.

Total convective heat transfer
= Advection + Diffusion

Convective Heat Transfer

Fluid-solid convection

The total convective heat transfer is expressed by Newton's law of cooling, in which a convective coefficient relates the rate of heat transfer with the solid's surface area and the temperature difference between the surface and the fluid (away from the surface):

$$Q_f = h A_s \left(T_s - T_f \right)$$

The convective heat transfer coefficient is application-dependent: it is influenced by flow conditions (velocity, direction, type), problem geometry (system shape / size), etc.
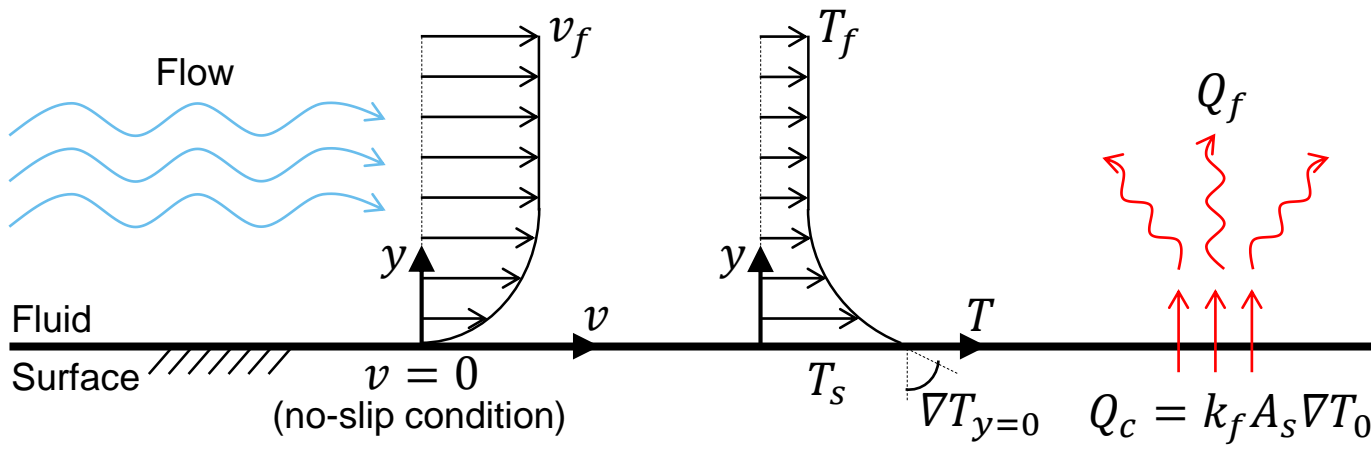
In the interface, heat is transferred by conduction. Then, it is propagated through the fluid by diffusion and advection.

$$h A_s \Delta T = k_f A_s \nabla T_0$$

$$h = \frac{k_f \nabla T_0}{\Delta T}$$

$Q_c = k_f A_s \nabla T_0$

The *Nusselt* number (*Nu*) is then used to allow a general description of convection.

Nusselt number

Dimensionless number of the ratio between the total convective heat transfer and a fictitious pure conduction situation (as if the fluid was completely still).

$$N_u = \frac{Q_f}{Q_c} = \frac{hA_s\Delta T}{k_f A_s \Delta T/l} = \frac{hl}{k_f}$$

$$\begin{cases} \text{Stagnant fluid} \rightarrow N_u = 1 \quad \text{(heat diffusion only)} \\ \text{Laminar flow} \rightarrow N_u = 1{\sim}10 \\ \text{Turbulent flow} \rightarrow N_u = 10^2{\sim}10^3 \quad \text{(heat advection dominates)} \end{cases}$$

Analogous to the *Biot* number, but employing the thermal conductivity of the fluid, instead of the solid, thus being a comparative measure of the advection and diffusion contributions to the total convective heat transfer within the fluid.

T_2

advection

l

diffusion

T_1
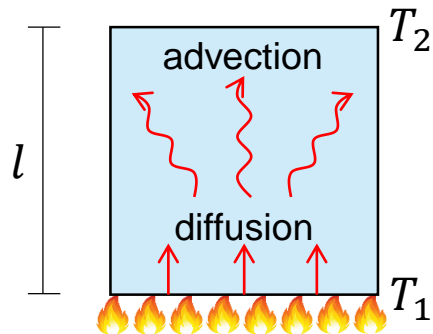
Total convection: $Q_f = hA_s\Delta T$

Pure conduction: $Q_c = \dfrac{k_f}{l}A_s\Delta T$

$$N_u = \frac{hl}{k_f} = \frac{\nabla T_0}{\Delta T/l}$$

The temperature profile, thus the gradient, is not known in most of the situations.

There are many correlations to relate N_u with flow conditions, problem geometry, etc. Most of them involve the *Reynolds* and *Prandtl* numbers, and the average porosity.

Convective Heat Transfer

***Reynolds* number**

Dimensionless number of the ratio between inertial and viscous forces in a fluid flow.

Helps to predict the flow characteristics in different scenarios.

Depends on specific application properties: flow velocity and characteristic length.

$$R_e = \frac{\rho_f v_f l}{\mu_f}$$

Low R_e → Viscous forces dominate
(laminar flows)

High R_e → Inertial forces dominate
(turbulent flows)

***Prandtl* number**

Dimensionless number of the ratio between momentum and thermal diffusivities.

Depends only on fluid properties: heat capacity, viscosity and conductivity.

$$P_r = \frac{c_f \mu_f}{k_f}$$

$P_r \ll 1$ → Thermal diffusivity dominates
(heat diffuses quicker)

$P_r \gg 1$ → Momentum diffusivity dominates
(velocity diffuses quicker)

Convective Heat Transfer

Convective heat transfer correlations

Predominant correlations for particle-fluid convection in DEM simulations (Peng, 2020):

Authors	Correlation	Conditions
Ranz & Marshall (1952)	$$N_u = 2 + 0.6 R_e^{1/2} P_r^{1/3}$$	$R_e = 1.0 \sim 10^4$ $P_r = 0.6 \sim 380$
Whitaker (1972)	$$N_u = 2 + \left(0.4 R_e^{1/2} + 0.06 R_e^{2/3}\right) P_r^{2/5} \left(\frac{\mu_f}{\mu_{fs}}\right)^{1/4}$$	$R_e = 3.5 \sim 7.6 \times 10^4$ $P_r = 0.71 \sim 380$ $\mu_f / \mu_{fs} = 1.0 \sim 3.2$
Gunn (1978)	$$N_u = (7 - 10\varepsilon + 5\varepsilon^2)\left(1 + 0.7 R_e^{1/5} P_r^{1/3}\right) +$$ $$(1.33 - 2.4\varepsilon + 1.2\varepsilon^2) R_e^{7/10} P_r^{1/3}$$	$R_e < 10^5$ $R_a < 10^9$ All P_r
Li & Mason (2000)	$$N_u = \begin{cases} 2 + 0.6\varepsilon^m R_e^{1/2} P_r^{1/3} & R_e < 200 \\ 2 + \varepsilon^m \left(0.5 R_e^{1/2} + 0.02 R_e^{4/5}\right) P_r^{1/3} & R_e < 1500 \\ 2 + 0.000045\varepsilon^m R_e^{9/5} & R_e > 1500 \end{cases}$$	$m = 3.50 \rightarrow$ dilute $m = 4.75 \rightarrow$ dense $P_r = 0.7 \sim 1.0$ $\varepsilon = 0.35 \sim 1.0$

μ_{fs}: Fluid's dynamic viscosity at surface's temperature (may be assumed as $\mu_{fs} = \mu_f$)

Convective Heat Transfer

Convective heat transfer correlations

- Most of the correlations are empirical or semi-empirical.

- In DEM simulations, most of them are for flows past a single sphere.

- A given correlation is not generally applicable to different problems and / or conditions, so it must be selected with due care.

- The correlations can be grouped based on their application to systems with different solid concentration: dense systems, dilute systems, pneumatic systems.

- The correlation by Ranz & Marshall has become the foundation for many succeeding models. It is the most common for smooth spheres and has been employed in both dilute and dense DEM systems.

- The correlation by Gunn is mainly for relatively dilute systems.

- The correlation by Li & Mason was developed for pneumatic transport.

- Many other correlations are available in the literature, although not widely used as the ones listed above.

Convective Heat Transfer

Flowing fluid through DEM particles

To account for the convective heat transfer between particles and the surrounding fluid, a suited correlation is employed to determine N_u for the specific problem conditions.

The value of N_u is then used to estimate the convection coefficient and the rate of heat transfer (for spheres, the characteristic length is taken as the diameter: $l_i = 2R_i$):

$$N_u(R_e, P_r, \varepsilon) \quad \rightarrow \quad h_i = \frac{N_u k_f}{2R_i} \quad \rightarrow \quad Q_{f,i} = h_i A_{s,i}(T_f - T_p) = \frac{N_u k_f}{2R_i} A_{s,i} \Delta T = 2\pi R_i k_f N_u \Delta T$$

The basic properties needed for the fluid and for characterizing the flow are:

- Fluid properties: k_f, ρ_f, c_f, μ_f
- Flow properties: v_f, l_i (for R_e)

These properties should be known locally, around each particle. For simplicity, in most DEM simulations, their given values are assumed to hold for all particles.

Convective Heat Transfer

Stagnant fluid around DEM particles

For nearly stationary particles within a stagnant interstitial fluid, R_e vanishes.

This leads to a constant value of N_u ($N_u = 2$, in most correlations).

The fact that $N_u \neq 1$ in this case indicates that advection still plays a role even though the fluid is considered still around the particle. The advection effect is due to the natural convection that occurs near the surface and is considered by the correlation formulas.

$$N_u = 2 \quad \rightarrow \quad h_i = \frac{k_f}{R_i} \quad \rightarrow \quad Q_{f,i} = \frac{k_f}{R_i} A_{s,i}\left(T_f - T_p\right) = 4\pi R_i k_f \Delta T$$

In both cases of flowing and stagnant fluid, an assumption is that the effect of particle rotation is neglected for computing N_u, and thus h_i and $Q_{f,i}$.

Furthermore, a 1-way thermal coupling between the interstitial fluid and the particles is normally assumed: the fluid temperature affects the particles temperature, by means of convective heat transfer, but not the opposite way.

4 – Radiative Heat Transfer

Radiative Heat Transfer

Thermal radiation

Heat transfer by emission of electromagnetic waves, as a consequence of thermal agitation of molecules, without the need for a transmitting medium.

All heated bodies (above 0K) emit thermal radiation.

Heat transfer occurs among the surface of the bodies.

For a black body*, the radiation power can be expressed by Stefan-Boltzmann law:

$$\sigma = 5.6703.\,10^{-8}\ [W/m^2 K^4]$$

$$I = \sigma T_s^4$$

$$Q_{rbb} = A_s I$$

All incident radiation is absorbed

Blackbody Radiator

Emitted Radiation is only a function of Radiator's Temperature
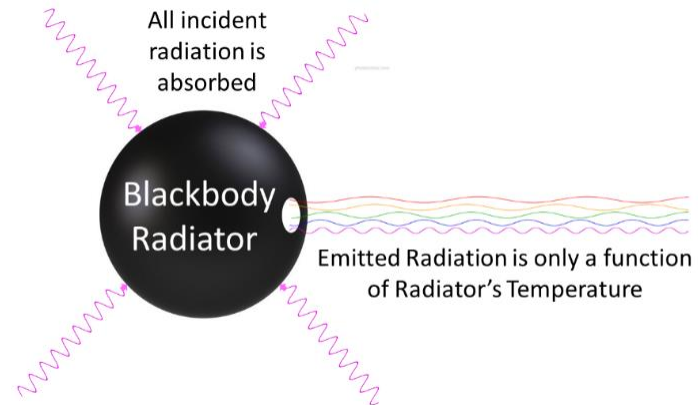
* Hypothetical body that absorbs all incident thermal radiation that falls on its surface, and emits radiation on the same rate (perfect absorber and emitter).

Radiative Heat Transfer

Net radiation with surrounding environment

The radiation emitted by real surfaces is calculated as a fraction of the black body radiation, given by an emissivity coefficient ($\epsilon = 0 \sim 1$), which is a surface property:

$$Q_{out} = \epsilon Q_{rbb} = \epsilon A_s \sigma T_s^4$$

The incident radiation (irradiation) from the surroundings (whose average temperature is T_e) is partially reflected, absorbed and transmitted. The absorbed fraction is given by an absorptivity coefficient which, under the "grey body" assumption, is equal to the emissivity coefficient:

$$Q_{in} = \epsilon A_s \sigma T_e^4$$

The net rate of radiative heat transfer to a body is then:

$$Q_r = \epsilon A_s \sigma (T_e^4 - T_s^4)$$

Net radiation with other surfaces

The irradiation that falls on an object's surface may come from any other surface to which the analyzed object is exposed to.

The net radiative heat transfer from one surface to another depends on their shapes and relative position, which is accounted by view factors $F_{i \to j}$.
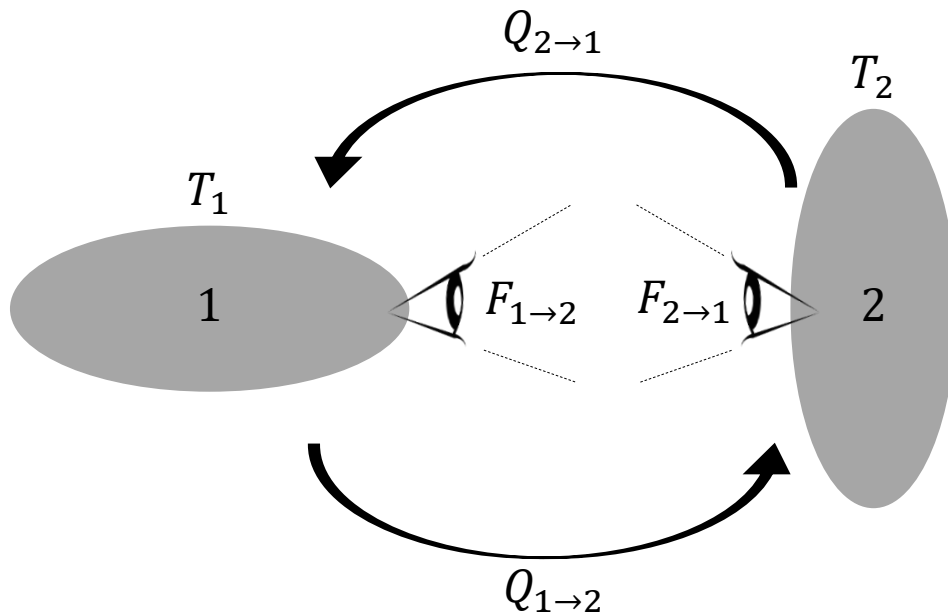
$$Q_1 = Q_{2 \to 1} - Q_{1 \to 2}$$

$$Q_1 = \epsilon F_{2 \to 1} A_{s,2} \sigma T_2^4 - \epsilon F_{1 \to 2} A_{s,1} \sigma T_1^4$$

By reciprocity: $F_{1 \to 2} A_{s,1} = F_{2 \to 1} A_{s,2}$

$$Q_1 = \epsilon F_{1 \to 2} A_{s,1} \sigma (T_2^4 - T_1^4)$$

Radiative Heat Transfer

DEM radiation models

Because of the 4th-order dependency on the temperature, the amount of heat transfer increases significantly as temperature increases, but becomes relevant only at high temperatures (typically > 700K – Zabrodsky, 1966).
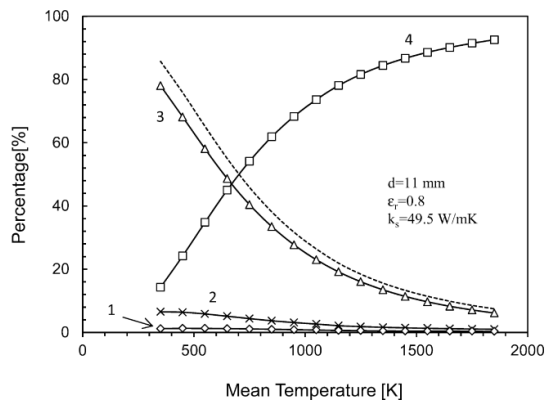
Figure 13. Effect of mean bed temperature on the relative contributions of the heat transfer mechanisms to the overall heat transfer: line 1, heat conduction Q_{nsfs}; line 2, heat conduction Q_{csfs}; line 3, heat conduction Q_{css}; line 4, the solid–solid radiation between particle surfaces; dashed-line, the percentage of total conduction.   Cheng et al (2013)
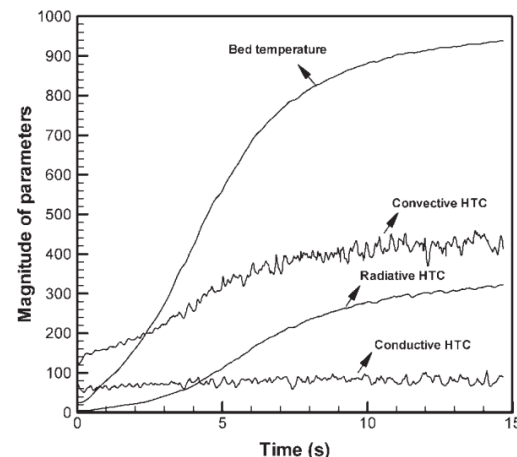
Figure 16. Thermal behavior of bed particles under the condition of gas inlet temperature 1,000°C, and superficial velocity 3.2 m/s.   Zhou et al (2009)

Radiation is more challenging and computationally expensive to be considered than other heat transfer mechanisms, thus it is generally neglected at lower temperatures.

In solid-liquid systems, it disappears, so it is only considered in solid-gas systems (Kunii & Smith, 1960).

DEM radiation modeling approaches

Continuum	Discrete
Simplified approach based on average local properties of the model. It assumes a representative environment temperature around each particle to which the particle is exposed. There is no need to compute view factors (computationally cheaper).	Computes the heat transfer between the surfaces of individual particles based on the solution of view factors. It provides more accurate results but it is more computationally expensive. (currently not covered in this presentation)
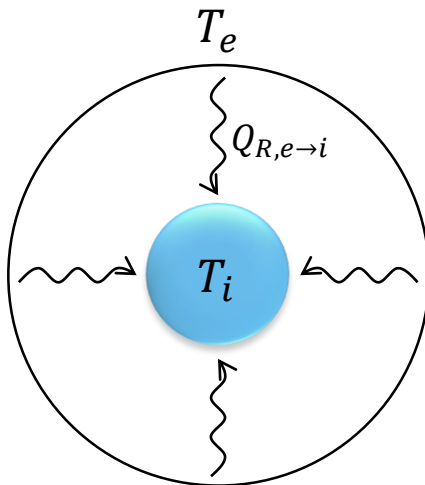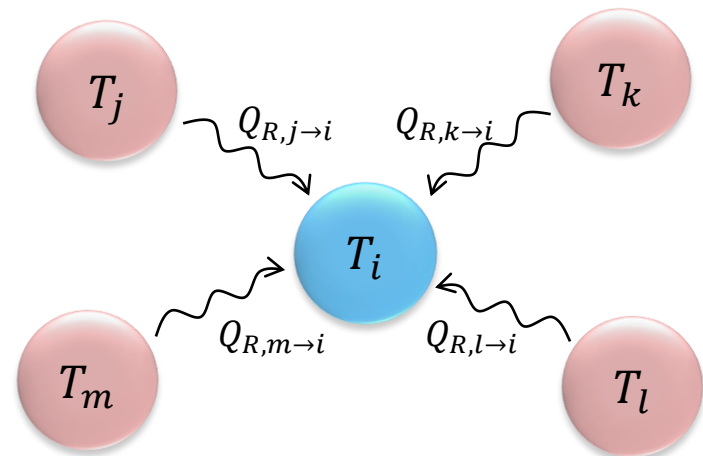
Radiative Heat Transfer

Continuum model

A spherical volume of radiative influence is defined around each particle (the radius of the spherical domain is normally set as $3R_i$).

An environment temperature is assumed for the enclosing surface, taken as the volume averaged temperature of the n_p surrounding particles and the fluid as:

- Zhou et al (2009):
$$T_e = \varepsilon T_f + (1 - \varepsilon) \frac{1}{n_p} \sum_{j=1}^{n_p} T_j$$

- Krause et al (2017):
$$T_e = \left(\frac{\sum_j \epsilon_j A_j \sigma T_j^4 / 2}{\sum_j \epsilon_j A_j \sigma / 2} \right)^{1/4}$$

It assumes that if the centroid of another particle lies within the spherical domain, the half surface of this particle is considered.

The radiative heat transfer between each particle and the surrounding environment is:

$$Q_{r,i} = \epsilon_i A_{s,i} \sigma \left(T_e^4 - T_i^4 \right)$$

5 – Heat Generation

Heat Generation

Besides heat flow by conduction, convection and radiation due to temperature gradient, heat might also be generated by several mechanisms:

- Energy dissipation
    - → Friction between particles
    - → Kinetic energy loss during collision
- Phase change
- Chemical reactions
- Biological activity

Al-Arkawazi (2017) concluded that the contribution of heat generated by energy dissipation mechanisms in static and fluidized beds is very small compared to the heat transfer mechanisms:
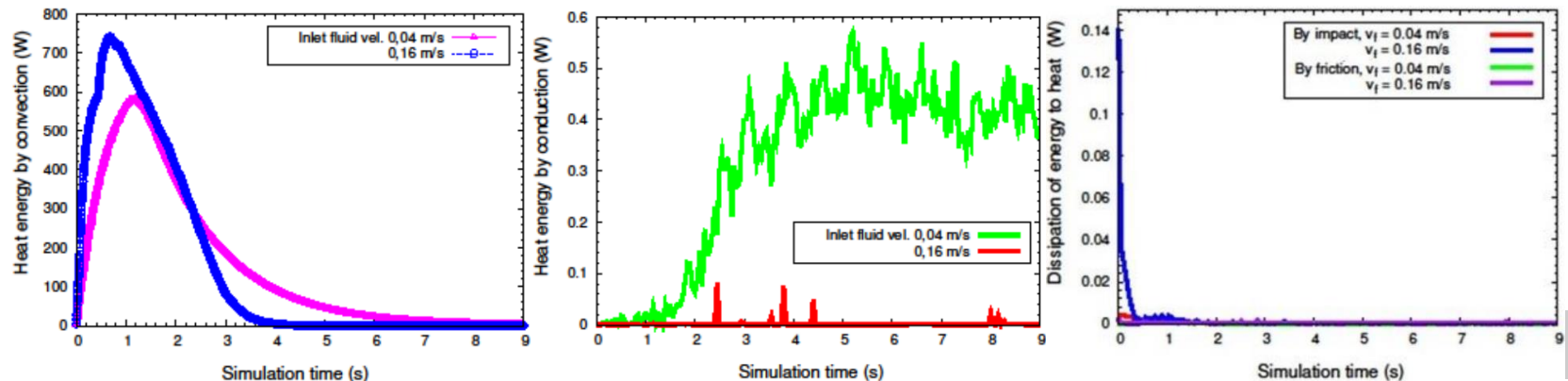
Heat Generation by Friction

Energy dissipated by friction between particles is converted to heat.
Some ways of modeling this type of heat generation are as follows:

- Nguyen et al (2009), Al-Arkawazi (2017):

$$Q_g = \hat{\mu}|v_t F_n| \begin{cases} \hat{\mu} & \rightarrow \quad \text{Dynamic friction coefficient} \\ v_t & \rightarrow \quad \text{Tangential (sliding) relative velocity between particles} \\ F_n & \rightarrow \quad \text{Normal contact force} \end{cases}$$

- Rojek (2014):

$$Q_g = \chi|v_t F_t| \begin{cases} \chi & \rightarrow \quad \text{Fraction of friction work converted to heat } (0 \leq \chi \leq 1) \\ v_t & \rightarrow \quad \text{Irreversible part of the relative tangential velocity} \\ F_t & \rightarrow \quad \text{Tangential contact force} \end{cases}$$

The frictional heat is generated at the contact point and absorbed by both particles.

The amount of heat absorbed by each particle is given by a partition coefficient ψ:

$$Q_g = Q_{g,i} + Q_{g,j} \qquad \begin{cases} Q_{g,i} = \psi_i Q_g \\ \\ Q_{g,j} = (1 - \psi_i) Q_g \end{cases}$$

Several formulas have been proposed for computing the partition coefficient :

Váradi et al (1996): $\quad \psi_i = \dfrac{k_i}{k_i + k_j}$

Rojek (2014): $\qquad \psi_i = \dfrac{e_i}{e_i + e_j} \qquad e = \sqrt{\rho c k}$

(thermal effusivity)

$$\psi_i Q_g$$

$$Q_g$$

$$(1 - \psi_i) Q_g$$
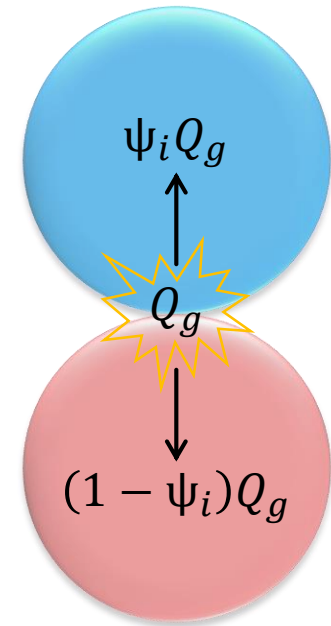
If both particles have the same material:

$$\psi_i = 0.5$$

Appendix A – Contact Mechanics

Contact Mechanics

Effective parameters used for the contact between 2 spheres

$$\bar{R} = \left(\frac{1}{R_i} + \frac{1}{R_j} \right)^{-1} = \frac{R_i \cdot R_j}{(R_i + R_j)} \qquad \bar{m} = \left(\frac{1}{m_i} + \frac{1}{m_j} \right)^{-1} = \frac{m_i \cdot m_j}{(m_i + m_j)}$$

$$\bar{k} = \left(\frac{1}{k_i} + \frac{1}{k_j} \right)^{-1} = \frac{k_i \cdot k_j}{(k_i + k_j)} \qquad \bar{E} = \left(\frac{1 - (\upsilon_i)^2}{E_i} + \frac{1 - (\upsilon_j)^2}{E_j} \right)^{-1}$$

A wall can be treated as a particle with $R_{\text{wall}} = m_{\text{wall}} = \infty$

Hertz theory

Accurately describes the elastic behavior of spheres in contact or colliding, therefore it is normally used for the heat transfer models by contact conduction.

Models the contact of elastic and smooth solids based on the linear theory of elasticity (Hertz, 1882; Timoshenko & Goodier, 1951; Johnson, 1985).

Assumptions:

- Perfectly elastic bodies (strains are sufficiently small to consider linear elasticity).

- Perfectly smooth surfaces (i.e. frictionless – only normal pressure).

- Parabolic profile of stresses over the contact area, which is assumed as circular.

- The contact area must be small compared to the dimensions of each body and to the relative radii of curvature of each surface.

Contact Mechanics

Contact parameters – static loading by Hertz

The case of 2 spheres brought and kept into contact by a normal force F_n.

Contact radius:

$$R_c^{\text{htz}} = \left(\frac{3}{4} \frac{F_n \bar{R}}{\bar{E}} \right)^{1/3} = \sqrt{\bar{R} \delta_n}$$

Particle displacement: (DEM overlap)

$$\delta_n = \frac{\left(R_c^{\text{htz}} \right)^2}{\bar{R}} = \left(\frac{9}{16} \frac{F_n^2}{\bar{R}\bar{E}^2} \right)^{1/3}$$

P.S. The relationship between normal force and overlap is:

$$F_n = K_{HZ} \delta_n^{3/2} \qquad K_{HZ} = \frac{4}{3} \bar{E} \sqrt{\bar{R}}$$

Contact Mechanics

Contact parameters – quasi-static loading by Hertz

The collinear impact between elastic frictionless bodies follows the static Hertz theory.

Hertz theory was developed for static contact, but it is valid for collisions as long as the impact velocity is small compared to the speed of bulk elastic waves.

It is quasi-static in the sense that the deformation is assumed to be restricted to the vicinity of the contact area and to be given by the static theory.

Gives the solution of the dynamic system for normal collision: $\bar{m}\ddot{\delta}_n + K_{HZ}\delta_n^{3/2} = 0$

Maximum contact radius and overlap:
$$R_c^{\max} = \left(\frac{15}{16}\frac{\bar{m}\bar{R}^2}{\bar{E}}\dot{\delta}_n^{0\,2}\right)^{1/5} \qquad \delta_n^{\max} = \frac{(R_c^{\max})^2}{\bar{R}} = \left(\frac{15}{16}\frac{\bar{m}}{\sqrt{\bar{R}}\bar{E}}\dot{\delta}_n^{0\,2}\right)^{2/5}$$

Total collision time:
$$t_c = 2.87\left(\frac{\bar{m}^2}{\bar{R}\bar{E}^2\dot{\delta}_n^0}\right)^{1/5} \qquad \text{where} \qquad t_c^{\max} = \frac{t_c}{2}$$

Contact parameters – geometry based

Independent of the contact model and overlap magnitude, computed based on the overlap geometry, which is assumed in DEM.

The contact radius for overlapping circles / spheres is: (Musser 2011; Zohdi 2013; Weisstein)

$$R_c^{\text{geo}} = \sqrt{R_i^2 - \left(\frac{R_i^2 - R_j^2 + {d_{ij}}^2}{2d_{ij}}\right)^2}$$

or

$$R_c^{\text{geo}} = \frac{1}{2d_{ij}} \sqrt{4{d_{ij}}^2 R_i^2 - \left({d_{ij}}^2 - R_j^2 + R_i^2\right)^2}$$
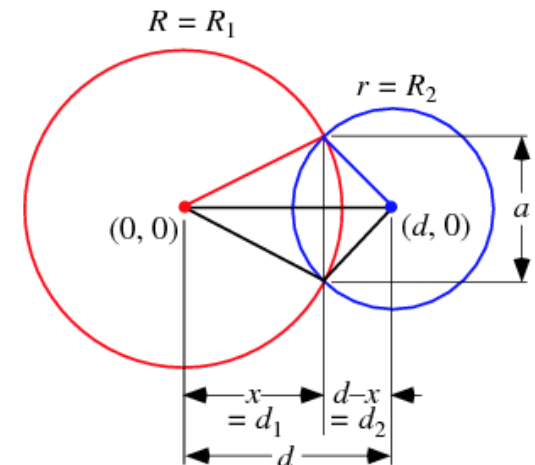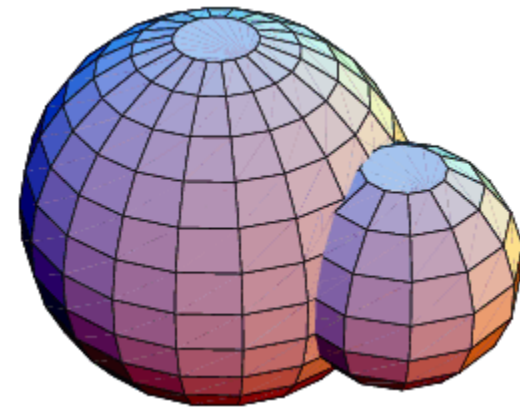
Nomenclature & Bibliography

Nomenclature

Symbols

a, b, c	Auxiliary parameters for indirect conduction [K/W]
ac	Thermal accommodation coefficient [-]
A	Auxiliary parameters for indirect conduction [-]
A_c	Contact area [m^2]
A_g	Surface area exposed to gas [m^2]
A_l	Surface area exposed to liquid [m^2]
A_n	Face area of Voronoi polyhedron [m^2]
A_p	Cross-section area of thermal pipe [m^2]
A_s	Surface area [m^2]
B	Auxiliary parameter for indirect conduction [-]
B_i	*Biot* number [-]
c	Specific heat capacity [J/(kg.K)]
c_f	Specific heat capacity of fluid [J/(kg.K)]
c_g	Specific heat capacity of gas [J/(kg.K)]
C	Correction coefficient [-]
$C_1 - C_4$	Correlation parameters [-]
$d_f(r)$	Distance for conduction through fluid [m]
d_g	Molecule diameter of gas [m]
d_{ij}	Distance between centroids of particles *i* and *j* [m]
$d_p(r)$	Distance for conduction within particle [m]
d_{pw}	Distance between centroid of particle *i* and wall [m]
dQ	Elementary rate of heat transfer [W]
D	Distance from particle centroid to separation plane [m]
E	Young modulus [Pa]
$\bar{E}$	Effective Young modulus [Pa]
$F_{i \rightarrow j}$	View factor from *i* to *j* [-]
F_n	Normal contact force [N]
F_t	Tangential contact force [N]
F_o	Fourier number [-]
G	Shear modulus [Pa]
h	Convective heat transfer coefficient [W/(m^2.K)]
I	Radiation emissivity power [W/m^2]
k	Thermal conductivity [W/(m.K)]
$\bar{k}$	Effective thermal conductivity [W/(m.K)]
$\tilde{k}$	Average thermal conductivity [W/(m.K)]
k_B	Boltzmann constant [m^{2}kg/(s^{2}K)]
k_f	Thermal conductivity of fluid [W/(m.K)]
k_g	Thermal conductivity of gas [W/(m.K)]
k_g^*	Modified thermal conductivity of gas [W/(m.K)]
k_l	Thermal conductivity of liquid [W/(m.K)]
k_p	Thermal conductivity of particle [W/(m.K)]

Nomenclature

K_n	Normal spring stiffness coefficient [N/m]
K_{hz}	Hertzian spring stiffness coefficient [N/m]
l	Characteristic length [m]
l_g	Characteristic length of heat flux in gas [m]
l_l	Characteristic length of heat flux in liquid [m]
m	Mass [kg]
$\bar{m}$	Effective mass [kg]
M	Auxiliary parameter for indirect conduction [m]
n_p	Number of particles [-]
N_u	*Nusselt* number [-]
P_g	Pressure of gas [Pa]
P_r	*Prandtl* number [-]
Q	Net rate of heat transfer [W]
Q_c	Rate of heat transfer by conduction [W]
Q_{cpfp}	Rate of heat transfer by conduction due to contact particle-fluid-particle [W]
Q_{cpp}	Rate of heat transfer by conduction due to particle-particle contact [W]
Q_{npfp}	Rate of heat transfer by conduction due to non-contact particle-fluid-particle [W]
Q_{pfp}	Rate of heat transfer by conduction through the fluid between particles [W]
Q_{pfw}	Rate of heat transfer by conduction through the fluid between particle and wall [W]
Q_e	Rate of heat transfer by external source [W]
Q_f	Rate of heat transfer by fluid convection [W]
Q_g	Rate of heat generated [W]
$Q_{i \to j}$	Rate of heat transfer from *i* to *j* [W]
Q_r	Rate of heat transfer by radiation [W]
Q_{rbb}	Rate of heat transfer by radiation of a black-body [W]
r	Radial coordinate [m]
r_c	Radius of the isothermal core of particle [m]
r_{ij}	Equivalent radius of the double tapered cone [m]
r'_{ij}	Plane size to circumvent the inconsistency induced by different particle sizes [m]
r_{in}	Auxiliary parameters for indirect conduction [-]
r_{out}	Auxiliary parameters for indirect conduction [-]
r_{sf}	Radius of the intersection between the tapered cone and the particle [m]
r_θ	Radial coordinate at the base of tapered cone [m]
R	Radius [m]
$\bar{R}$	Effective radius [m]
R_a	Rayleigh number [-]
R_c	Radius of contact area [m]

Nomenclature

R_C^{cor}	Corrected radius of contact area [m]
R_C^{geo}	Current radius of contact area according to geometric arguments [m]
R_C^{htz}	Current radius of contact area according to Hertz theory [m]
R_C^{max}	Maximum radius of contact area during a collision [m]
R_{cap}	Radius of surface area exposed to liquid bridge [m]
R_e	*Reynolds* number [-]
R_f	Upper boundary radius for indirect conduction [m]
R_k	Maximum radius between two particles [m]
R_l	Minimum radius between two particles [m]
R_p	Radius of particle [m]
S	Min. separation distance for indirect conduction [m]
t	Time [s]
t_c	Total time expected for collision [s]
T	Temperature [K]
T_e	Temperature of surrounding environment [K]
T_f	Temperature of fluid [K]
T_p	Temperature of particle [K]
T_s	Temperature of surface [K]
T_w	Temperature of wall [K]
T_θ	Temperature at the base of tapered cone [K]

U	Thermal energy [J]
v	Velocity [m/s]
$\bar{v}$	Velocity vector [m/s]
v_f	Velocity of fluid [m/s]
v_t	Tangential relative velocity [m/s]
V_{ij}	Volume the double tapered cone [m³]
$\bar{x}$	Position vector [m]
$x_{min,max}$	Auxiliary parameter for indirect conduction [-]
Y_1, Y_2	Auxiliary parameter for indirect conduction [-]

Greek letters

α	Thermal diffusivity [m²/s]
β	Auxiliary parameter for indirect conduction [m]
γ	Dimensionless radius of particle [-]
δ_f	Surrounding fluid layer of particle [m]
δ_i^{min}	Auxiliary parameter for indirect conduction [m]
δ_i^{max}	Auxiliary parameter for indirect conduction [m]
δ_n	Normal overlap [m]
$\dot{\delta}_n$	Normal overlap velocity [m/s]
$\ddot{\delta}_n$	Normal overlap acceleration [m/s²]
δ_n^{max}	Maximum normal overlap in a collision [m]

Nomenclature

$\dot{\delta}_n^0$ Normal overlap velocity at impact [m/s]

Δ Increment of a quantity [-]

∇ Gradient of a quantity [-]

ε Porosity (void fraction) [-]

ϵ Emissivity coefficient [-]

ζ Ratio of specific heat capacities [-]

θ Angular coordinate [rad]

θ_0 Angle between normal direction and tapered cone [rad]

θ_1 Lower boundary angle for indirect conduction [rad]

θ_2 Upper boundary angle for indirect conduction [rad]

θ_c Angle between normal direction and contact point [rad]

Λ Auxiliary parameter for indirect conduction [-]

μ Dynamic viscosity [Pa.s]

$\hat{\mu}$ Dynamic friction coefficient [-]

μ_f Dynamic viscosity of fluid [Pa.s]

μ_{fs} Dynamic viscosity of fluid at surface temperature [Pa.s]

μ_g Dynamic viscosity of gas [Pa.s]

υ Poisson ratio [-]

ρ Density [kg/(m^3)]

ρ_f Density of fluid [kg/(m^3)]

σ Stefan-Boltzmann constant [W/(m^2.K)]

φ Filling angle of liquid bridge between particles [rad]

χ Fraction of friction work converted to heat [-]

ψ partition coefficient of friction heat generation [-]

ω Molecular mean free-path [m]

Subscripts

cr Critical value of a quantity

e Surrounding environment property

f Fluid property

g Gas property

i, j Particle indexes

k, l Max./Min. quantity between *i* and *j*

l Liquid property

p Particle property

$real$ Quantity computed with real material properties

s Surface property

w Wall property

Superscripts

t Time step index

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