Discrete element simulation of Slumping mode of granular particles and their heat transfer in a rotating cylinder

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Abstract: ***A discrete element method (DEM) study is conducted to investigate the mixing and heat-transfer characteristics of spherical particles under slipping mode and flow regimes of a rotating tumbler. In this paper, heat transfer in rotating drums operated in a slipping mode is assessed. The focus is on direct heating operations at low to medium temperatures, where thermal radiation is unimportant. It is shown that heat transfer from the covered wall to the particle bed is the dominant mechanism in supplying heat to the bed. . If heat is supplied to the boundaries of the particle bed rapidly, and macroscopic particle mixing is rapid, then heat transfer within the bed may be controlled by either or both of particle –wall heat transfer and heat conduction within individual particles depending upon the physical properties of particles. Although theoretical analyses are principally used in this work. This paper addresses heat conduction in granular systems under slumping mode in a rotating cylinder. The influence of material properties on the contact heat transfer coefficient between the covered wall surface and the solid bed was investigated.***

Keywords: DEM simulation, Granular materials, Slumping Mode, Heat transfer.

1. Introduction

Rotating Cylinder play a noticeable role in the processing of granular material in chemical industries in an extensive variety of physical processes, including size reduction, waste reclamation, agglomeration, solid mixing, drying, heating, cooling, etc. The general use of rotating cylinder is also caused by its ability to handle various feedstock, from slurries to granular materials, and to activate in distinct environments. Rotary cylinder are the most usually used mixing devices in metallurgical and catalyst industries. Rotary dryers play an important role in many industrial applications, such as chemistry, metallurgy and materials science, and mineral industries, and food processing [23], [25]. It is important to recognize the mixing characteristics and heat transfer presentation. DEM models is the study of mixing in various amalgamation systems including rotating drum[5], Particle transport is vital and happens in two directions: transverse and axial. Particle transport in the transverse direction is comparatively uniform, while particle transport in the axial direction may diverge with different residence time.

Heat transfer in particulate materials distresses a wide variety of applications ranging from multi-phase reactors to kilns and calciners. Heat transport through flowing particulate materials is an essential component of modern

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technologies such as heterogeneous catalytic reactors, high performance cryogenic insulation, construction material, and powder metallurgy. In catalyst industrial, heat transfer through granular media happens in the drying and calcination stages. In addition to that, a comparison between a detailed 2D model resolving the gas phase and the uniform temperature model was performed by [27] who investigated the heating of coal particles in a rotating kiln. They indicated an over-prediction of the heating rate in the simulations that assumed a homogeneous particle temperature. In a recent work a 1D radial temperature model was applied by [32]. Figueroa [13] used thermal particle dynamics to examine the interplay between transient heat transfer and particle mixing in rotating tumblers, determining the effect of mixing and heating rates on granular materials under different tumbler shapes and operating parameters, such as rotating rate and filling level. The model used for heat transmission between two particles was the same as the one used by [5]. Over the last 50 years, there has been a sustained interest in the role of system parameters and in the mechanisms of heat transfer between granular media and the boundary surfaces in fluidized beds [3],[12],[15], dense phase chutes, hopper sand packed beds [33],[37],[6],[36],[31],[38], dryers and rotary reactors and kilns [17],[26],[24],[4]. The DEM was initially developed to simulate the mechanical response of a granular bed. However, it can easily be prolonged to study other physical properties such as heat transfer [18], [5], [16], [21].

In order to recover the performance of the procedures taking place inside the rotating cylinder, a better understanding of the transport phenomena in the granular medium inside the rotating cylinder is required. During particle motion, solid particles inside the cylinder experience numerous processes like heat exchange, drying, heating, chemical reaction etc. Hence it is very essential to have a fundamental understanding of the processes occurring inside a rotating cylinder, so that it can be designed to function under optimum process conditions.

2. NUMERICAL MODEL

The discrete element method (DEM), originally developed by Cundall and Strack [10], [11], has been used successfully to simulate chute flow [11], heap formation [19], hopper discharge [39], [30], blender segregation [40], [35],[20]and flows in rotating drums [29],[40]. In the present study DEM is used to simulate the dynamic behavior of granular materials in a rotating drum (calciner).Granular material is considered here as a collection of frictional elastic spherical particles. The equation of motion for each particle are derived from Newton's law of classical Newtonian dynamics. These include a system of equations for the translational motion of centre of gravity and rotational motion around the centre of gravity for each particle in the granular medium. Translational motion of the centre of gravity of a particle *i* can be fully described by a system of equations [1].

$$m_i \frac{d^2 x_i}{dt^2} = m_i a_i$$

$$= F_i$$

Rotational motion of the particle *i* around the centre of gravity can be fully described by the following systems of equations [1].

$$I_i \frac{d^2 \theta_i}{dt^2} = T_i$$

Each particle may interact with its neighbors or with the boundary only at contact points through normal and tangential forces. The forces and torques acting on each of the particles are calculated as

$$F_i = F_{i,contact} + F_{i,gravity} + F_{i,external}$$

$$T_i = T_{i,contact} + T_{i,fluid} + T_{i,external}$$

Thus, the force on each particle is given by the sum of gravitational, inter-particle (normal force and tangential force) and external forces). The corresponding torque on each particle is the sum of the total torque caused by anti-symmetric fluid drag forces, the summation of torques caused by other external forces and the summation of all the torques caused by the contact forces between the particles. The normal forces are calculated using the “spring dashpot model”), which allows colliding particles to overlap slightly. The normal interaction force is a function of the overlap. The contact force F_{ij} can be expressed as the sum of normal and tangential components,

$$F_{ij} = F_{n,ij} + F_{t,ij}$$

Contact force between the spherical particles are modelled as spring, dash-pots and a friction slider. Spring accounts for elastic repulsion (*k*).Dash-pot accounts for damping effect (η). Friction slider express the tangential friction force in the presence of normal force (μ).

The contact forces between particles depend on the overlap geometry, the properties of the material and the relative velocity between the particles in the contact area. Hence in the perfect contact model, it is required to describe the effects of elasticity, energy loss through internal friction and surface friction and attraction on the contact surface for describing the contact force calculations.

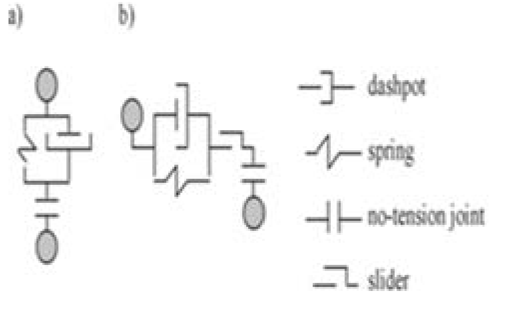

Figure 1.Contact model for DEM simulations in the (a) normal and (b) tangential directions.

The normal component of contact force between particles can be expressed as the sum of elastic repulsion, internal friction and the surface attraction forces.

$$F_{n,ij} = F_{n,ij,elastic} + F_{n,ij,viscous}$$

Normal elastic repulsive force is based on the linear Hooke's law of a spring with a spring stiffness constant $k_{n,ij}$ and is given by the expression,

$$F_{n,ij,elastic} = K_{n,ij} h_{ij} n_{ij}$$

Normal energy dissipative force is dissipated during real collisions between particles and, in general, it depends on the history of impact. A very simple and popular model is based on the linear dependency of force on the relative velocity of the particles at the contact point with a constant normal dissipation coefficient γ_n and is expressed as

$$F_{n,ij,viscous} = -\gamma_n m_{ij} v_{n,ij}$$

The tangential component force model depends on the normal force and normal displacement. Further the model for static friction must include energy dissipation, because perpetual oscillations in tangential direction will be obtained during the time of static friction. In the literature two major approaches can be found to represent tangential contact forces namely; global and complex models. Global models describe all the phenomena of the tangential force through a single expression. Complex models describe static and dynamic friction by separate equations and the Coulomb criteria. Of course, the continuous particle interaction models require special models for tangential forces. The tangential force $F_{t,ij}$ being divided into parts of static friction or dynamic friction. When the tangential force $F_{t,ij}$ is larger than the Coulomb-type cut-off limit, dynamic friction predominates. When $F_{t,ij}$ is lower than the limit, the model of static friction force $F_{t,ij,static}$ must be implemented. Such an approach can be modelled by

$$F_{t,ij} = -t_{ij} \min\left(|F_{t,ij,static}|, |F_{t,ij,dynamic}|\right)$$

Dynamical frictional force can be described as

$$F_{t,ij,dynamic} = -\mu |F_{n,ij}| t_{ij}$$

Static frictional force is the sum of the tangential spring and energy dissipation force

$$F_{t,ij,static} = F_{t,ij,spring} + F_{t,ij,dissipation}$$

3. GRANULAR BED MOTION IN THE TRANSVERSE PLANE

The motion of a bed of granular solids in the transverse plane of a rotated cylinder can take different forms, as described by [14]. As the cylinder rotation speed is increased from zero, six distinct modes of bed behavior viz., slipping, slumping, rolling, cascading, cataracting and centrifuging are observed, as shown schematically in Figure 2.

3.1 Slipping Mode

At very low rotational speeds, particularly when the friction between the granular bed and the cylinder wall is low, the granular bed performs as a rigid body. The bed motion is observed to take one of two forms (i) the granular bed remains at rest and the granular solid continuously slides at the wall, or (ii) the granular solid repeatedly moves upward with the cylinder until the bed surface reaches a maximum inclination and then slips at the wall back to a minimum inclination and then resumes rotation.

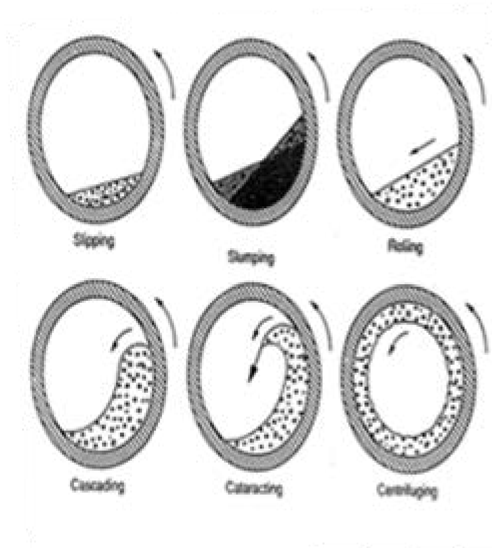

Figure 2: Schematic view of the different modes of solids motion.

3.2 Slumping Mode

In this mode, the granular solid is raised like a rigid body by the cylinder wall such that the feeling of the bed surface increases unceasingly until it reaches an upper angle of repose, then separates from the upper surface of the bed, and falls as a discrete avalanche toward the lower half of the bed. Next the avalanche the inclination of the surface of the granular solid drops to an angle of repose that is less than the static angle of repose of the granular solid. The slumping frequency is experiential to increase with increasing rotation speed, finally leading to the rolling mode. The change between the slumping and rolling modes of bed motion is not always obviously defined, rather the bed behaviour is found to go through a transition in which the bed changes randomly between rolling and slumping behaviour.

3.3. Rolling Mode

The majority of the bed rotates as a rigid body about the cylinder axis at the same rotation speed as the cylinder wall. On the bed surface there appears a thin layer of continuously falling particles forming a plane free surface that is inclined at the dynamic angle of repose of the granular solid to the horizontal plane. Solid particles mix more effectively in the rolling mode. In the rolling mode, bed material can be divided into two distinct regions, namely a 'passive region or plug flow region' where the particles are carried upward by the cylinder wall, and a relatively thin 'active region or cascading layers. In the passive region, granular mixing is negligible and the mixing mainly occurs in the active region. At higher mixer rotational speeds, the continuous flow rolling regime is obtained, in which a thin layer of particles flows down the free surface while the remaining particles rotate as a fixed bed. Transverse mixing in this event depends on the dynamics and outcomes from the shearing and collisional diffusion inside the layer.

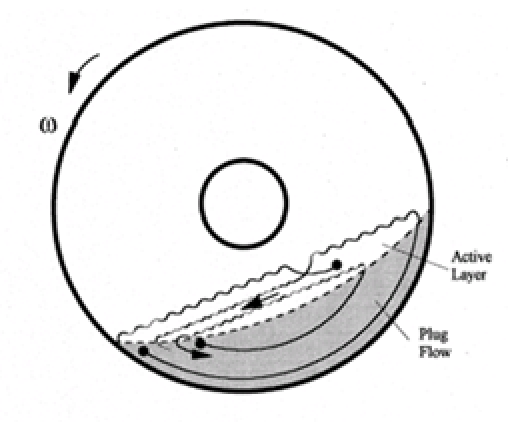

Figure 3. Rolling bed motion: top plane- active layer; bottom plane –plug flow (non-shearing region), (Boateng [1993])

3.4. Cascading Mode

As the rotation speed is increased additional, the particles in the upper corner of the rolling bed are lifted higher before detaching from the cylinder wall, and the bed surface assumes a crescent shape in the cylinder cross-section. This mode of material motion is termed as cascading mode.

3.5. Cataracting Mode

On further increasing the rotational speed, centrifugal forces become increasingly significant in the motion of particles along the bed surface, the curvature of the cascading surface becomes highly pronounced and particles are projected into the freeboard space from the upper corner of the bed.

3.6. Centrifuging Mode

At a Froude number of unity, the granular solid is restrained to the inner wall of the cylinder by centrifugal forces. According to [22], the critical rotational speed at which a particle at the cylinder wall starts centrifuging can be calculated from the equation where g is the acceleration due to gravity and 0 is the diameter of the cylinder.

4. Simulation of Slumping Modes of the Granular Solid Bed

As the rotational velocity of the cylinder was increased further, the slumping of the granular bed commences. For most of the time, the entire granular bed rotates at the same rotational velocity, thus undergoing solid body rotation. Further an avalanche is triggered when the bed surface reaches the static angle of repose Θ_s . During the avalanche, material from the upper part of the bed surface slides rapidly down. At the end of avalanche period the bed surface was inclined at a lesser angle Θ_d called the dynamic angle of repose. Solid body rotation of the whole bed ensues, until the surface inclination again reaches the angle Θ_s when avalanching occurs and the cycle is repeated. Davidson et al (2000) has given the following relationship for characterizing the slumping cycle time:

$$t_{13} = t_{12} + \frac{(\Theta_s - \Theta_d)\pi}{180\omega}$$

Where t_{12} the avalanche time, t_{13} is the total cycle time and Ω is the rotational velocity of the cylinder. The schematic view of one slumping cycle is shown in the Figure 4 (a) to 4(c).

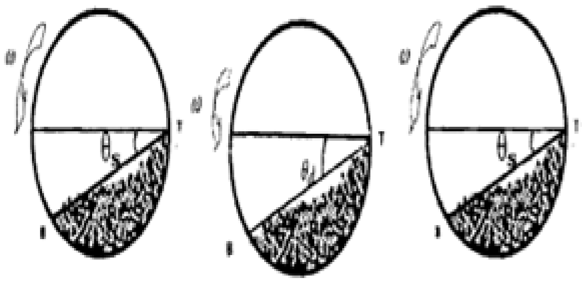

Figure: 4(a) to(c): Cyclic slumping or avalanching
(a) Initial stage of a slump at an angle Θ_s ,
(b) Final stage of a slump at an angle Θ_d and
(c) Initial stage of the next slump at an angle at Θ_s

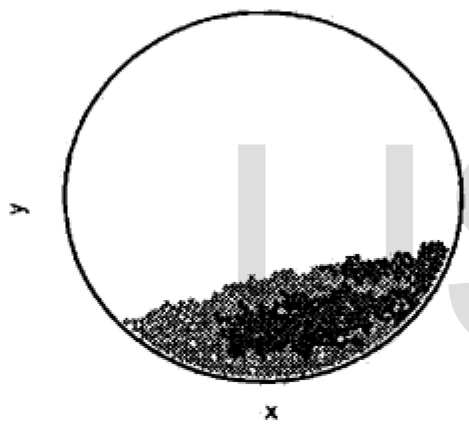

Figure 5. The granular solid bed profile at the beginning of avalanching in slumping mode

It has been shown by Henein [14] that the slumping frequency is dependent on the rotational speed, particle size and cylinder diameter. The slumping mode of the granular solid bed motion is shown in Figures 5 where the rotational velocity of the cylinder is kept at 10 rpm. Figure 6 and 7 shows the velocity profile of the granular solid bed at the beginning or avalanching of the surface particles and the end of the avalanching of the particles respectively, in the slumping mode.

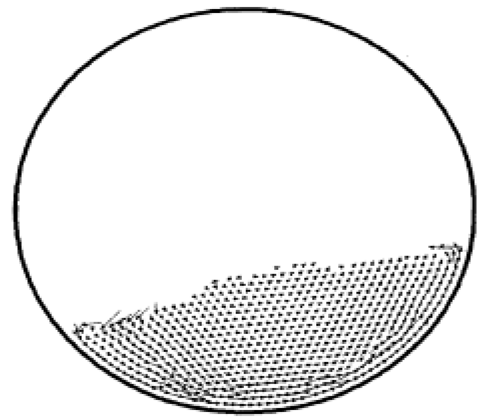

Figure 6. Vector plot of the granular solid bed during solid body rotation in slumping mode.

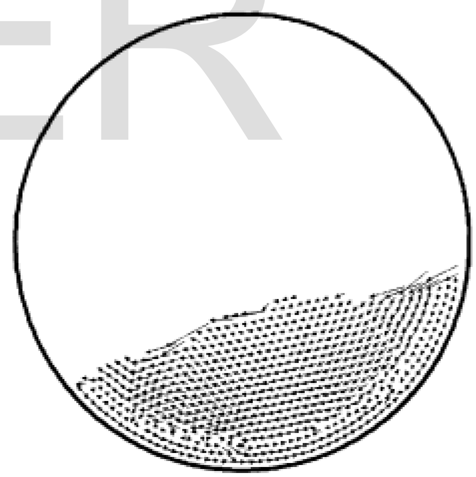

Figure 7. Vector plot of the granular solid bed at the beginning of avalanching in slumping mode.

The trajectory of a single particle in the slumping mode is shown in figure 8, which shows that, the particles will have much movement. The corresponding kinetic energy distribution and the dynamic angle of repose variation are shown in Figures 9 and 10. The angles Θ_s , and Θ_d are found to be approximately 17.5^0 and 15.1^0 and the avalanching duration is found to be around 3s and the predicted cycle time based on equation turns out to be

3.3s which agrees with the predicted value of 4s given by Davidson [18] for the same process parameters.

5. Heat transfer in a Rotating Drum

Heat transfer always happens from a region of high temperature to another region of lower temperature and heat transfer stops when the two mediums touch the same temperature. There are three elementary modes of heat transfer: Conduction, Convection, and Radiation. More recently, [34] employed a discrete element method–computational fluid dynamics (DEM–CFD) technique to simulate realistic heat transfer in rotary kilns varied from convection-dominated to conduction-dominated heat transfer. Figueroa [13] used thermal particle dynamics to examine the inter play between transient heat transfer and particle mixing in rotating tumblers. The mechanisms of heat transfer between granular solids and boundary surfaces of the processors have been experimentally investigated by a number of researchers. Many of these studies have proposed empirical correlations for bed temperature, thermal conductivity, and heat transfer coefficients for a range of operating parameters [7].

Conduction heat transfer always happens over the contacted area between particles or between particles and wall. Generally, such conduction heat transfer due to elastic deformation comprises two mechanisms: conduction due to particle-particle static contact (particularly common in a packed bed) and conduction due to particle-particle collision, which happens in a moving or fluidized bed. For conduction due to particle-particle static contact, the equation proposed by [28] and modified by [8] is adopted. Thus, the heat flux Q_{ij} through the contact area between particles *i* and *j* can be calculated according to the equation below:

$$Q_{i,j} = \frac{4r_c(T_j - T_i)}{\left(1/K_{pi} + 1/K_{pj}\right)}$$

For particle-wall static or collision contact, a wall can be preserved as a particle with an infinite diameter and mass, as usually used in the DEM work. Its properties are presumed to be the same as particles. The algorithm is used to examine the evolution of the particle temperature in the rotating cylinder. This numerical model is developed based on following assumptions:

1) Interstitial gas is neglected.
2) Physical properties such a heat capacity, thermal conductivity and Young Modulus are considered to be constant.
3) During each simulation time step, temperature is uniform in each particle.
4) Boundary wall temperature remains constant.

The major computational tasks at each time step are as follows:(i) add/delete contact between particles, thus updating neighbour lists, (ii) compute contact forces from contact properties, (iii) compute heat flux using thermal properties (iv) sum all forces and heat fluxes on particles and update particle position and temperatures, and (v) determine the trajectory of the particle by integrating Newton’s laws of motion (second order scalar equations inn three dimensions). Hence the 5th order Gear predictor-corrector scheme [2] is used to solve the equations, which is stable for second-order differential equations

6. Slumping Mode of heat transfer by the particles.

Initially, particles are loaded into the system in a non-overlapping fashion and allowed to reach mechanical equilibrium under gravitational settling. Subsequently, the vessel is rotated at slumping mode, and the evolution of the position and temperature of each particle in the system is recorded as a function of time. The curved wall is considered to be frictional. To minimize the finite size effects the flat end walls are considered frictionless and not participating in heat transfer.

A parametric study was conducted by varying thermal conductivity, particle heat capacity, Kinetic energy, vessel fill ratio, and vessel speed of the Rotating drum. A cohesive granular material is considered to examine the effect of thermal properties and the speed of the vessel. To visually track the evolution of particle temperature, color-coding was used. Particles with temperature less than 350K are coloured blue; those with temperature in between 350 and 550K are considered cyan. Those with temperature in between 550 and 750K are considered green and for temperatures between 750 and 950K are considered yellow. Those particles with temperature more than 950K are coloured red.

7. Result and Discussion

7.1. Effect of thermal conductivity

Three values of thermal conductivity of the solid material are considered: 96.25, 192.5, 385W*/mK*. The cylinder is rotated at the speed of 20 rpm. As the heat source is the wall, the particle bed warms up from the region in contact to the wall. In slumping mode particle–wall contacts cause the transport of heat from the wall to the particle bed. With subsequent particle–particle contacts, heat is transported inside the bed. The blue core signifies the mass of particles at initial temperature. As conductivity increases, the system exhibits faster heating.

Uniformity in the bed temperature increases with conductivity until the end of five revolutions. Finally the bed with higher conductivity rapidly reaches a thermal equilibrium with the isothermal wall, where all the particles in bed reach the wall temperature and there is no more heat transfer.

7.2. Effect of Kinetic energy

The simulation was continued till all the particles came to rest; that is until the total kinetic energy of the system becomes negligible. Heat changes the speed of moving particles of matter. Transferring heat to a substance increases the movement or kinetic energy of the particles in that substance. Transferring heat from a substance slows down the movement of the particles in that substance. That is, the kinetic energy of the particles decreases.

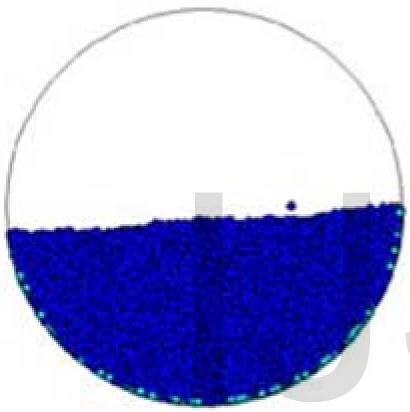

Figure 11. Particles at initial temperature

7.3. Effect of heat capacity

The other main thermal property of a material is heat capacity. Three values of heat capacity of the granular material are considered: 172, 344 and 688 J/kg K, while keeping the thermal conductivity constant at 385W/mK. Once again, the cylinder is rotated at the speed of 20 rpm. Bed temperatures are estimated as a function of time. The variability in the bed temperature is larger for the material with lower heat capacity until 2 revolutions, but at the end of five revolutions, more uniform temperature is observed for the material of lower heat capacity.

7.4. Effect of vessel speed

In order to examine the effect of vessel speed, the most cohesive granular system is rotated at different rpm, for thermal transport properties constant and equal to: k_s = 385W/*mK* and *Cp* = 172 J/kgK. The higher vessel speed applies a higher shear rate to the granular system, causing significant differences in flow behavior, evident in the different dynamic angle of repose of the bed at each rotational speed. On a per revolution basis, slower speed caused higher temperature rise. At slower speeds, each particle has a more prolonged contact with the heated wall, which contributes to the rapid rise in the temperature. The effect of speed disappears as the average bed temperatures for all the cases follows nearly identical trends. While the temperature of the bed is more uniform at slower speeds on a per revolution basis. This effect almost disappears on the real time basis.

7.5. Effect of fill ratio

Three different fill levels are simulated using different number of particles. Once again, the vessel is rotated at 20 rpm. Particle's thermal transport properties remain constant at k_s=385W/mK and Cp=172J/kgK. The change in average bed temperature with time is shown as a function of the fill ratio. As expected, the granular bed with lower fill fraction heats up faster. Faster mixing is achieved for the lower fill fraction case, which causes rapid heat transfer from the vessel wall to the granular bed. The temperature is more uniform for lower fill fraction at the end of the five revolutions.

8. Conclusion

This study investigated the mixing and thermal conduction of granular particles in tumblers using DEM and incorporate thermal conduction between contact particles. Increasing rotation speed decreases heat transfer and temperature uniformity on a per revolution basis but the effect disappears on a per-time basis. Cylinder exhibit faster heating of the granular bed for material with higher conductivity and lower heat capacity. Hence this work is directed towards a theoretical investigation based on Discrete Element Method (DEM) and Thermal Particle Dynamics (TPD) for predicting the mixing and heat transfer phenomena in the slumping mode of granular solids bed in the transverse direction of the horizontal cylinder to elucidate the relationship between the operating parameters of the rotating cylinder geometry and physical properties of the granular solid.

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