

Review of DEM Models to Simulate Granular Beds in Rotary Kilns

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Abstract - Rotary kilns are thermal reactors widely used in industrial processes such as calcination, sintering, drying, and thermal reduction of granular materials or fluids. These devices consist of slightly inclined metallic cylinders that rotate slowly around their longitudinal axis. The combination of rotation and gravity allows bed material to flow from the feeding point to the discharge point. The mass flow is given by the longitudinal movement, while the transversal displacement mixes the bed material. Regarding the transverse motion of the granular bed, the Froude number (Fr) is used to characterize three main flow regimes: cascading, cataracting, and centrifugal. The objective of this paper is to describe the functioning of Discrete Element Method (DEM) models for simulating granular beds in rotary kilns. DEM enables high-fidelity simulation of both mechanical and thermal behavior by resolving particle-scale interactions. However, it entails a high computational cost, which scales with the number of particles. This work also examines alternative modeling approaches—such as zero-dimensional, one-dimensional, and multiphysics models—and compares their accuracy, computational demands, and applicability, providing a clear assessment of the advantages and limitations of DEM relative to continuum and hybrid frameworks.

Keywords: Rotary kiln, Discrete Element Method (DEM), granular flow, heat transfer, thermal modeling.

1. Introduction

Rotary kilns are used in industry to carry out a variety of processes such as calcination, sintering, or pyrolysis, where controlled exposure of the material to high temperatures is required [1]. This kind of equipment, consisting of an inclined and rotating hollow cylinder, allow the gradual displacement of the solid material from the inlet to the outlet, while being in contact with a high-temperature source activates the desired transformation of the bed material. The net longitudinal flow along the kiln is directly related to the equipment's processing capacity, while the transverse movement through the cross-sectional area is related to the mixing capacity. The transverse motion can be characterized by the Froude number (Fr), which allows identifying whether the bed is in a cascading, rolling, or centrifuging regime [2]. These regimes have a determining influence on the thermal distribution within the bed. Models based on the Discrete Element Method (DEM) are particularly useful for simulating all these flow regimes with high fidelity, capturing the bed's heterogeneity. However, their main limitation lies in the high computational cost, which increases with the number of simulated particles.

Another key parameter in thermal modeling is the Biot number (Bi) [3], which is defined as the ratio between the internal and external thermal resistance to heat transfer. At the level of the entire bed, if the Biot number is low ($Bi < 0.1$), it is considered that the internal resistance to heat transport is negligible compared to the external one, implying a uniform temperature in the bed. In this case, zero-dimensional models can be used, representing the bed as a whole without spatial thermal gradients [4]. If the Biot number of the bed is high ($Bi > 1$), significant thermal gradients exist within the bed, requiring spatially resolved modeling. In this scenario, the use of models based on the Discrete Element Method is essential, as it allows capturing the thermal and mechanical heterogeneity of the granular bed. At the particle level, when the Biot number for particles is low, the internal temperature is uniform, which constitutes an important simplification commonly used in DEM models. On the other hand, DEM models that account for internal thermal gradients require discretization of the particle domain [5]. Respect to the thermal process, the heat transfer from the source of energy can be both internally transmitted through the central axis or externally transmitted via the kiln wall [6, 7]. A general heat transfer model for rotary kilns includes three key components: particle–particle interactions, particle–wall interactions, and how the source energy is transmitted to the bed.

The present article aims to provide a comprehensive review of the DEM models used to simulate granular beds in rotary kilns. The different approaches and techniques used to model the dynamics and heat transfer in these systems will be analyzed, as well as the limitations and challenges associated with simulating complex processes in rotary kilns.

2. Modeling of Rotary Kilns Using the Discrete Element Method

The simulation of granular bed behavior in rotary kilns using the Discrete Element Method requires the integrated modeling of three essential components: (1) the granular bed, (2) the kiln wall, and (3) the thermal interactions between the bed, the wall, and the heat source [4]. The granular bed, composed of individual particles in motion, must be modeled with accurate physical and dynamic properties to faithfully capture both the longitudinal flow—directly related to processing rate—and the transverse motion, which governs particle mixing and thermal exposure. The kiln wall acts not only as a mechanical boundary that guides bed movement but also plays a critical role in heat transfer, particularly in externally heated configurations. The thermal interactions among the bed, the wall, and the heat source must be explicitly incorporated to compute the temperature distribution within the bed. A DEM model for rotary kilns can be generally described as below.

2.1. DEM Modeling of Particles' Motion

The simulation of granular bed dynamics in rotary kilns using the Discrete Element Method relies on an accurate description of particle motion, governed by Newton second law and numerical integration schemes [12, 13, 14, 15]. This section presents a brief review of the three principal DEM modeling frameworks: (1) Molecular Dynamics (MD), (2) Event-Driven method (ED), and (3) Contact Dynamics (CD).

2.1.1. Molecular Dynamics Modeling

In rotary kilns, the granular bed consists of particles that interact with each other and with the walls of the rotating cylinder. The translational equation of motion for a particle i interacting with N different particles j is given by:

$$m_i \frac{\partial^2 \vec{r}_i}{\partial t^2} = \sum_{j=1, j \neq i}^N \vec{F}_{ij} \quad (1)$$

Where $\vec{r}_i$ is the position vector of particle i in space, m_i its mass, and $\vec{F}_{ij}$ is the net interacting force between particle i and j . This force includes normal and tangential contact interactions. The angular velocity is obtained similarly from the torque balance [8]. The normal force F_n can be modeled as a simple linear spring-damper [9] or by using a Hertz contact model [10]. The linear model corresponds to:

$$F_n = \begin{cases} K_n \delta_n + C_n \delta_n \dot{\delta}_n & \delta_n > 0 \\ 0 & \delta_n \leq 0 \end{cases} \quad (2)$$

The term $K_n \delta_n$ is the elastic component, where K_n is the elastic constant [N/m] and δ_n is the overlap between particles i and j , defined as:

$$\delta_n = R_i + R_j - |\vec{r}_i - \vec{r}_j| \quad (3)$$

Where R_i and R_j are the radius of the particles, and $|\vec{r}_i - \vec{r}_j|$ is the distance between their centers. $\delta_n > 0$ indicates that the particles are in contact and compressing (overlapping). In a rotary kiln, this term ensures that particles do not penetrate excessively during collisions. The term $C_n \delta_n \dot{\delta}_n$ represents the dissipative (viscous) component, where C_n is the normal viscous damping constant [kg/s], and $\dot{\delta}_n$ is the rate of change of compression, calculated as the relative normal velocity between the particles at the contact point:

$$\delta_n = -(\vec{v}_j - \vec{v}_i) \cdot \vec{e}_{ij}^n \quad (4)$$

Where $\vec{v}_j$ and $\vec{v}_i$ are the velocities of the particles, and $\vec{e}_{ij}^n = \frac{\vec{r}_j - \vec{r}_i}{|\vec{r}_j - \vec{r}_i|}$ is the unit vector in the normal direction [9]. This term simulates energy loss due to the inelasticity of collisions, a common phenomenon in granular materials where particles do not rebound perfectly (inelastic collisions).

The tangential force F_t is modeled similarly as a combination of an elastic and viscous component, adding the Coulomb friction criterion. The total tangential force F_t is given by:

$$F_t = -K_t \delta_t - C_t \delta_t \quad (5)$$

Where K_t is the tangential stiffness [N/m] and δ_t is the accumulated tangential displacement [m]. On the other hand, C_t is the tangential damping coefficient [N·s/m] and δ_t is the tangential relative velocity between the particles at the contact point [m/s]. The magnitude of the total tangential force is limited by Coulomb's friction law [8,11]:

$$|F_t| \leq \mu |F_n| \quad (6)$$

Where μ is the static friction coefficient ($\mu = \tan \phi$, where ϕ is the friction angle), and $|F_n|$ is the magnitude of the normal force.

2.1.2. Event Driven Modeling

The Event-Driven (ED) method is an alternative to the time-stepping MD approach, where the simulation progresses by detecting and resolving discrete collision events between particles or between particles with boundaries. Instead of continuous integration, the system evolves analytically between events, and time advances only when a collision occurs. This method provides high temporal accuracy for systems with low particle density and infrequent interactions. However, in dense granular flows—such as those found in rotary kilns—where multiple simultaneous contacts are common, the ED method becomes computationally prohibitive due to the exponential increase in event detection complexity. As a result, its application in industrial-scale kiln simulations is limited, and it is primarily used in fundamental studies of collisional dynamics or dilute flows [8].

2.1.3. Contact Dynamics

The Contact Dynamics (CD) method treats contacts as unilateral constraints with set-valued force laws, avoiding the use of artificial stiffness parameters. Instead of modeling contact as a deformable spring, CD enforces impenetrability and friction constraints through complementarity conditions, solving for contact forces implicitly at each time step. This approach is particularly effective for simulating rigid, frictional systems with persistent contacts, such as quasi-static or slow-flowing granular beds. However, due to its reliance on complex optimization algorithms, CD is not common in rotary kiln modeling [8].

2.2. DEM Modeling of Heat Transfer

The discrete frameworks for the granular bed have two parts: a dynamic model, which describes translational and rotational motion by using force interaction laws; and a heat transfer model, which includes conduction mechanisms between particles and, in some cases, thermal interaction with the surrounding gas (particle–gas), either by conduction or convection [16, 17]. The energy balance for a particle i in the bed can be simplified when the Biot number is less than 0.1. In this case,

the sensible heat of the particle depends only on a unique temperature T_i . The energy balance for a particle i includes the following heat flows depending on its location in the bed:

- Interior particles: these grains only receive thermal conduction from contact with neighboring particles ($Q_{cond,p-p}$).
- Surface particles: this kind of grain receives thermal conduction from contacts, plus superficial convection and radiation ($Q_{conv,p-a}$ and Q_{rad}).
- Particles in contact with the wall: these grains receive conduction from contacts plus an additional conductive flow from the wall ($Q_{cond,p-w}$).

The energy balance considering all the cases before can be written in a general form as [18, 19, 20,21]:

$$\rho_p c_p V_p \frac{\partial T_i}{\partial t} = Q_{cond,p-p} + Q_{conv,p-a} + Q_{rad} + Q_{cond,p-w} \quad (7)$$

Where:

$$Q_{cond,p-p} = \sum_{j \in C_i} H_{c,ij} (T_j - T_i) \quad (8)$$

Here, C_i represents the contacts of the particle i , while the thermal conductance coefficient $H_{c,ij}$ represents the rate of heat transfer between particles i and j . Depending on the specific interaction mechanism, $H_{c,ij}$ can be expressed as $H_{c,ij}^{s-s}$ or $H_{c,ij}^{s-g}$. $H_{c,ij}^{s-s}$ is a solid-solid coefficient based on the mechanical-elastic contact theory of Hertz [8]:

$$H_{c,ij}^{s-s} = 2k_p \left(\frac{3|F_n|r^*}{4E^*} \right)^{1/3} \quad (9)$$

Where k_p is the effective thermal conductivity between particle i and j , expressed in units of [W/(m·K)], r^* is the effective radius of the particles in contact and E^* is the effective elastic modulus. A solid-solid plus solid-gas conduction coefficient $H_{c,ij}^{s-g}$ also can be used [21,22]:

$$H_{c,ij}^{s-g} = \left(\frac{1}{R_c} + \frac{1}{R_g} \right)^{-1} \quad (10)$$

Here, R_c is the thermal constriction resistance and R_g is the resistance of a stagnant gas zone computed as:

$$R_c = \frac{1}{2k_p r^*} \quad (11)$$

$$R_g = \frac{l_g}{k_g A_g} \quad (12)$$

Where A_g is the cross-sectional area of the stagnant gas zone and l_g is the length of the stagnant gas zone. On the other hand [16,17]:

$$Q_{conv,p-a} = h_{conv} A_{se} (T_{a,\infty} - T_i) \quad (13)$$

$$Q_{rad} = q A_{pr} \quad (14)$$

Where h_{conv} is the convective heat transfer coefficient, expressed in units of $[W/(m^2 \cdot K)]$, A_{se} is the effective exposed surface area of the particle i , $T_{a,\infty}$ is the temperature of the gaseous environment, q is the absorbed radiation, expressed in units of $[W/m^2]$ and A_{pr} is the effective projected area of the particle perpendicular to the radiant flow.

Finally:

$$Q_{cond,p-w} = H_{c,iw} (T_{w,int} - T_i) \quad (15)$$

Where $T_{w,int}$ is the temperature of the wall and $H_{c,iw}$ is the thermal conductance coefficient between the particle and the kiln wall. This coefficient can be calculated by considering the thermal resistances of solid-solid contact and stagnant gas conduction, like those used for particle-particle conduction [21,22]:

$$H_{c,iw} = \left(\frac{1}{R_{cw}} + \frac{1}{R_{gw}} \right)^{-1} \quad (16)$$

Here, R_{cw} and R_{gw} are the resistances in the contact particle-wall and interstitial gas-wall, respectively.

2.3. Modeling of Thermal Interactions Between: Granular Bed, Kiln Wall, and Heat Source

The thermal model accounts for the three primary heat transfer mechanisms: radiation, conduction, and convection [17,18,19,20,29,33]. These mechanisms are critical for accurately simulating the complex thermal behavior of granular beds in rotary kilns. In the rotary kiln there is an exchange of energy between surfaces, particularly between the opening, the inner wall, and the granular bed. Conductive heat transfer occurs through direct physical contact between particles (particle–particle) and between particles and the kiln wall (particle–wall). Convective heat transfer accounts for the energy exchange between the granular bed and the surrounding gas phase, as well as between the kiln wall and the gas flow.

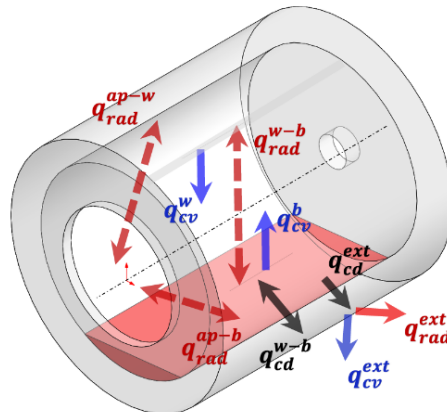


Fig. 1: Heat transfer mechanisms in rotary kiln [4].

Figure 1 illustrates the local thermal flows between the different components of the rotary kiln. These flows represent the heat flux density per unit area between the opening, the inner wall, the granular bed, and the external environment. Specifically, these flows are critical for understanding the coupled thermal behavior of rotary kilns, as demonstrated by experimental and numerical studies such as those conducted by Gallo [4]. In figure 1, q_{rad}^{ap-w} is the thermal flux by radiation between the opening and the inner wall, q_{rad}^{w-b} is the thermal flux by radiation between the inner wall and the granular bed, q_{rad}^{ap-b} is the thermal flux by radiation between the opening and the granular bed, q_{cv}^w is the thermal flux by natural convection from the inner wall to the environment, q_{cv}^b is the thermal flux by natural convection from the granular bed to the environment, q_{cd}^{w-b} is the thermal flux by conduction between the inner wall and the granular bed. On the other hand, q_{rad}^{ext} is the heat losses by radiation to the external environment, q_{cv}^{ext} is the heat losses by convection to the external environment and q_{cd}^{ext} is the heat losses by conduction to the external environment.

3. Modeling of Rotary Kilns Using Multiphysics Models

Multiphysics modeling represents a powerful approach for simulating the complex interactions between granular beds, fluid flow, and thermal behavior in rotary kilns. This method integrates Discrete Element Method (DEM) with Computational Fluid Dynamics (CFD) to capture the coupled dynamics of particles and surrounding fluids, as well as heat transfer mechanisms [5,29,30,31]. In multiphysics models, particle displacements are calculated using the linear momentum equations for viscous fluids, enabling detailed simulations of both particle motion and gas flow within the rotary kiln. Additionally, these models can resolve the internal temperature distribution within individual particles, particularly for larger grains where thermal gradients become significant. All the above allows researchers and engineers to explore complex phenomena such as particle-wall interactions, gas-solid coupling, and transient thermal effects, providing a comprehensive understanding of rotary kiln operations. Figure 2 illustrates a multiphysics model for granular beds in rotary kilns, showing how DEM and CFD are coupled to simulate the interaction between the granular bed and the surrounding gas phase. The model accounts for the rotational motion of the kiln, particle-particle interactions, and heat transfer through conduction, convection, and radiation. By combining DEM with CFD, multiphysics models offer unparalleled insight into the coupled thermal and mechanical behavior of granular beds, making them essential for advanced process optimization and design in rotary kilns.

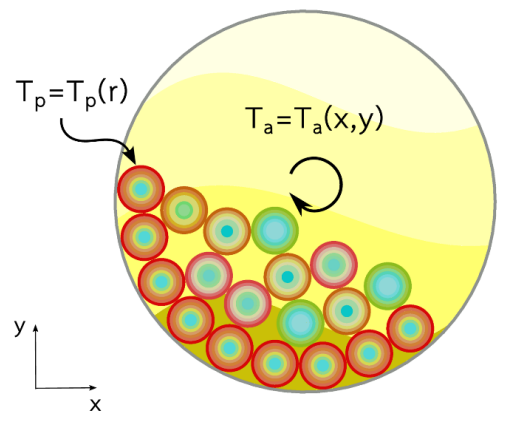


Fig. 2: Temperature field in rotary kiln by using a multiphysics model.

4. Advantages and disadvantages

Numerical models enable the simulation of rotary kilns under various operating conditions. Depending on the required level of complexity and detail, different approaches exist, each with advantages and disadvantages in terms of computational cost, accuracy and available software. Table 1 provides a comparative overview of the primary numerical models used in this field.

Table 1: Comparison of numerical models applied to rotary kilns.

	Computational cost		Precision		Commercial software
Zero-Dimensional Models [4,23]	✓ Low	Due to the simplicity of the equations and shorter computation time.	✗ Low	Low for large beds associated with a Biot number greater than zero ($Bi > 0$) of the bed.	Simple to program in open-source code. No expensive licenses required and accessible to users with basic knowledge.
One-Dimensional Models [23,24,25,26,27]	✓ Low	Solving ordinary differential equations of 1D.	🟡 Intermediate	Capture variations in one direction but ignore three-dimensional effects.	Simple to program in open-source code. Offers good flexibility for implementing custom equations.
Discrete Element Method (DEM) Models [31,32]	✗ High	High computational cost: - Standard hardware simulations (can simulate between 10^4 and 10^6 particles in 1–10 hours) - High-performance computing clusters (can simulate between 10^7 and 10^9 particles in 1 day to 1 week) - Complex model simulations (can simulate between 10^3 and 10^5 particles in hours to days or weeks).	✓ High	Very precise for particle motion if the particles are spherical and for particle-to-particle heat transfer.	Supported by specialized DEM software such as Rocky, YADE, or LIGGGHTS, which are optimized for particle simulations but require significant experience for parameter tuning and model validation.
Multiphysics Models [5,29,30,31]	✗ Very High	They combine DEM with CFD or other methods. They generally require clusters or supercomputers for realistic simulations.	✓ Very High	The combination of models offers the highest precision by considering both particles and the surrounding fluid.	Require advanced platforms like COMSOL Multiphysics or ANSYS Workbench, which allow coupling between different physics.

5. Conclusions

This review presents a comprehensive analysis of Discrete Element Method models for simulating granular beds in rotary kilns. DEM enables high-fidelity modeling of both mechanical and thermal behavior by resolving particle-scale interactions, making it particularly effective for capturing complex transverse flow regimes—such as cascading, cataracting, and centrifugal—that govern mixing and heat transfer.

The accuracy of DEM simulations depends on the proper representation of three key components: the granular bed, the kiln wall, and the thermal interactions between them. While Molecular Dynamics (MD)-based DEM is the most widely used approach due to its robustness and compatibility with multiphysics coupling, alternative methods such as Event-Driven (ED) and Contact Dynamics (CD) are limited to specific applications and are generally not scalable for industrial kiln simulations.

Accurate thermal modeling within the DEM framework requires a detailed representation of conduction, convection, and radiation. The Biot number serves as a critical criterion for determining the appropriate level of thermal resolution: for $Bi \leq 0.1$, the assumption of uniform particle temperature is valid and leads to computationally efficient models. For $Bi > 0.1$, internal thermal gradients must be resolved using advanced techniques such as multi-zone particle models.

A comparative analysis of modeling frameworks reveals a clear trade-off between computational cost and physical fidelity. Continuum models offer low computational cost but limited spatial resolution, while multiphysics DEM–CFD

models provide the highest accuracy at the expense of very high computational demands. DEM models alone occupy a strategic middle ground, offering detailed particle-level insights at a cost that, while high, is manageable with modern hardware and scalable algorithms. In summary, DEM-based models represent a powerful and versatile tool for analyzing, designing, and optimizing rotary kiln operations.

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