Numerical Modelling And Simulation Of Wet Ball Mills: A Review

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Abstract
Understanding the behavior of the mill load is crucial for optimizing the efficiency of wet ball mills. Computational simulations have played a significant role in unraveling the complex dynamics of wet ball mills, offering valuable insights into the underlying mechanisms. However, the literature lacks comprehensive reviews and summaries of the advancements made in modeling wet ball mills. This paper aims to bridge this critical gap by consolidating and presenting the major theoretical developments achieved in the past two decades in modeling and simulating wet ball mills. This review aims to comprehensively examine the coupling of Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM) as a numerical technique for simulating wet ball milling. The primary emphasis is on studies employing computational simulation techniques to investigate wet ball milling, with a focus on understanding the intricate interplay between the mill load, grinding media, slurry, and the mill structure. Firstly, particle motion and contact force models between particles, as well as the interaction forces in multiphase systems, as part of DEM and CFD theories are reviewed. Secondly, this paper discusses different ways of coupling CFD and DEM, including theoretical developments and applications, with a brief introduction to drag correlation models. Finally, the review highlights the main challenges currently faced by CFD-DEM and identifies exciting research topics for future studies. The study's findings illustrate the successful application of Discrete Element Method (DEM) in simulating the behavior of grinding media during wet milling. Additionally, Computational Fluid Dynamics (CFD) techniques, such as Smoothed Particle Hydrodynamics (SPH), have been utilized to model slurry behavior. Moreover, research indicates the feasibility of coupling CFD and DEM for simulating wet ball milling, although further investigation is required to enhance understanding in this area. It can be concluded that CFD-DEM is an effective method for simulating wet ball milling and offers a new perspective on understanding industrial processes and phenomena involving practical particle shapes. However, there are still aspects that require further investigation. By consolidating existing knowledge and identifying gaps in understanding, this review provides a roadmap for future research in this area.

Keywords: Discrete element modelling; Computational fluid dynamics; Wet ball mill; Coupled-CFD-DEM; Numerical Modelling; Slurry phase.

Introduction

Understanding the behaviour of the mill load is of utmost importance in enhancing the efficiency of wet ball mills. Wet ball milling is a widely used process in various industries, such as mineral processing, cement production, and pharmaceuticals [15]. Milling contributes significantly to the operational costs of mining operations, accounting for approximately 35% to 50% of the total expenses. Surprisingly, less

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than 10% of the energy supplied to a ball mill is effectively utilized for particle breakage [17, 9, 13, 30] This emphasizes the importance of thoroughly understanding the internal processes within a ball mill to optimize its efficiency. Even slight improvements in the design and operation of ball mills may lead to substantial cost savings. Therefore, it is understand how ball mills work to maximize their potential and improve their performance.

The performance of wet ball mills is influenced by factors such as the mill load, grinding media characteristics, slurry properties, and the mill structure. Traditional experimental methods have offered valuable insights into the behaviour of wet ball mills. However, their ability to capture the complex dynamics and interactions within the mill is limited. Experimental testing has the advantage of providing actual measurements under well-controlled operating conditions. However, it poses challenges due to the need for costly measurement instruments that must function effectively in the aggressive milling environment [28]. Computational simulations, specifically the coupling of Computational Fluid Dynamics (CFD) and Discrete Element Method (DEM), have revolutionized the study of wet ball milling by providing researchers with powerful tools to explore the underlying mechanisms in greater detail. This cutting-edge approach harnesses mathematical relationships translated into executable computer algorithms, enabling the comprehensive modeling of multiphysics systems. In the context of wet ball milling, this powerful approach involves replicating the movement of the ball charge, the behaviour of the liquid phase (slurry), and the interaction between the solid phase (grinding balls) and the liquid phase [15, 10]. By employing computational simulations, valuable insights into ball mills can be obtained at a fraction of the cost compared to experimental testing. This cost-effective approach offers researchers the opportunity to gain in-depth understanding and optimize the performance of ball mills without the need for expensive and time-consuming physical experiments.

Despite the progress made in modeling wet ball mills using computational simulations, there is a notable lack of comprehensive reviews and summaries on this topic. Such reviews are essential for consolidating the existing knowledge, identifying research gaps, and providing a direction for future studies. This literature review paper aims to address this critical gap by presenting a comprehensive overview of the major theoretical developments achieved in the past two decades in modeling and simulating wet ball mills.

The objective of this paper is to comprehensively review the existing published research that utilizes the coupling of CFD-DEM as a numerical technique for simulating wet ball milling. The focus is on studies that have employed computational simulation techniques to investigate wet ball milling and have contributed to understanding the intricate interplay between the mill load, grinding media, slurry, and the mill structure in the past decade. By analyzing and synthesizing the available literature, this review aims to provide a comprehensive understanding of the advancements made in modeling wet ball mills.

This review is organized as follows: Firstly, it summarizes the equations of particle motion and contact force models between particles, as well as the interaction forces in multiphase systems, as part of DEM and CFD theories. Understanding these fundamental equations is crucial for developing accurate numerical models of wet ball mills. Secondly, the review discusses different ways of coupling CFD and DEM, including theoretical developments and applications. It also provides a brief introduction to drag correlation models, which play a vital role in simulating the behaviour of the slurry within the mill. Finally, the review highlights the main challenges currently faced by CFD-DEM and identifies exciting research topics for future studies.

In conclusion, CFD-DEM has proven to be an effective method for simulating wet ball milling. It has provided valuable insights into the behaviour of the mill load, grinding media, slurry, and the mill structure. The coupling of CFD and DEM offers a new way of understanding industrial processes and phenomena involving practical particle shapes. However, there are still some aspects that require further investigation, such as the development of more accurate drag correlation models and the integration of additional complex phenomena. While some reviews have addressed the modeling of wet ball mills, they primarily focus on energy profiles and particle size reduction [56]. To the authors' best knowledge, there are no published comprehensive reviews specifically dedicated to the numerical modeling of wet ball mills. By consolidating the existing knowledge and highlighting the gaps in understanding, this review paper provides a roadmap for future research in the field of modelling and simulating wet ball mills. It is hoped that this review will inspire researchers to explore new avenues and contribute to further advancements in this area.

Methodology

A systematic and comprehensive approach was meticulously followed in the selection of literature for this review, aiming to provide a thorough understanding of the subject matter. The timeframe for the literature selection was explicitly defined to encompass the most pertinent and current studies available. The literature review strategy was intricately designed, involving systematic searches utilizing the well-regarded academic database Google Scholar. Special attention was directed towards utilizing keywords specifically related to "wet ball milling numerical simulation" and the coupling of Computational Fluid Dynamics with Discrete Element Method (CFD-DEM).

Articles included in this review were meticulously chosen from peer-reviewed journals based on their direct relevance to the topic and recency, specifically focusing on the application of CFD-DEM in wet ball milling processes. The primary emphasis was on research papers either published in English or translated to English within the last two decades to ensure the incorporation of the latest advancements and information in numerical simulations of wet ball milling processes. Noteworthy studies that made substantial contributions, even if published prior to the past 20 years, were also included to provide a comprehensive overview of the field.

This meticulous selection strategy was implemented to ensure a comprehensive, in-depth, and up-to-date review of the existing literature, encompassing developments and historically significant contributions in the domain of wet ball milling numerical simulations.

Numerical modelling of grinding media

The first step in the numerical modelling of ball mills is to define the behaviour of the grinding media. Discrete Element Method (DEM), a numerical technique extensively used in modelling the behaviour of solid particles in granular systems has been successfully applied to model the dynamic behaviour of grinding media. Thus, it has been possible to study mill charge dynamics, power draw, lifter design and grinding process of tumbling mills among other things [41,42,52,50,41,42,22,52,49,23,38,45,24]. The pioneering work on the Discrete Element Method (DEM) concept and its application to the study of molecular dynamics was spearheaded by [2]. Building upon this foundation, [16] significantly enhanced the theory of DEM through a meticulous exploration of numerical solutions for kinematic equations, enabling precise determination of both particle positions and orientations. The DEM technique is implemented by splitting dynamic events into discrete time steps. In doing so, finite particle displacements and rotations are numerically computed. Furthermore, DEM also applies contact models to represent collisions between particles [56,19]. The procedure is automated to perform the repetitive computations after each time step. The strength of the DEM technique resides in the ability to automatically perform contact detection for an assembly of particles and describe the motion of individual particles while allowing for particle-particle interactions [32].

Exploring the Theoretical Foundations of Discrete Element Method

In DEM analysis, the dynamics of the solid phase of a particulate system are governed by Newton's second law of motion applied at the centre of mass of each particle (Equation 1). Euler's second law of motion is used to describe changes in angular momentum (Equation 2).

$$m_i d\overrightarrow{v_i} = m_i \frac{d^2\vec{x}_i}{dt^2} = \sum_{j=CL_i} \vec{f}_{ij}^{\,p-p} + \vec{f}_i^{\,f-p} + \vec{f}_i^{\,ext} \qquad 1$$

$$I_i d\overrightarrow{\omega_i} = I_i \frac{d^2\overrightarrow{\omega}_i}{dt^2} = \sum_{j\in CL_i}\left(\vec{M}^t{}_{ij} + \vec{M}^r{}_{ij}\right) \; for\; j = 1, \dots, N \qquad 2$$

Where $\sum_{j=CL_i} \vec{f}_{ij}^{\,p-p}$ is sum of particle–particle interaction forces acting on particle i

$\vec{f}_i$ is the sum of different forces that act on the particle i

$\vec{M}_i$ is sum of different torques that act on particle i

x_i is the particle position

v_i is the translational velocity of particle

φ_j is the angular position.

ω_j is the rotational velocity of the particle

$\vec{f}_{ij}^{\,p-p}$ is particle-particle interaction forces.

$\vec{f}_i^{\,f-p}$ is fluid-particle interaction forces in multiphase systems. This term is ignored in pure DEM simulations.

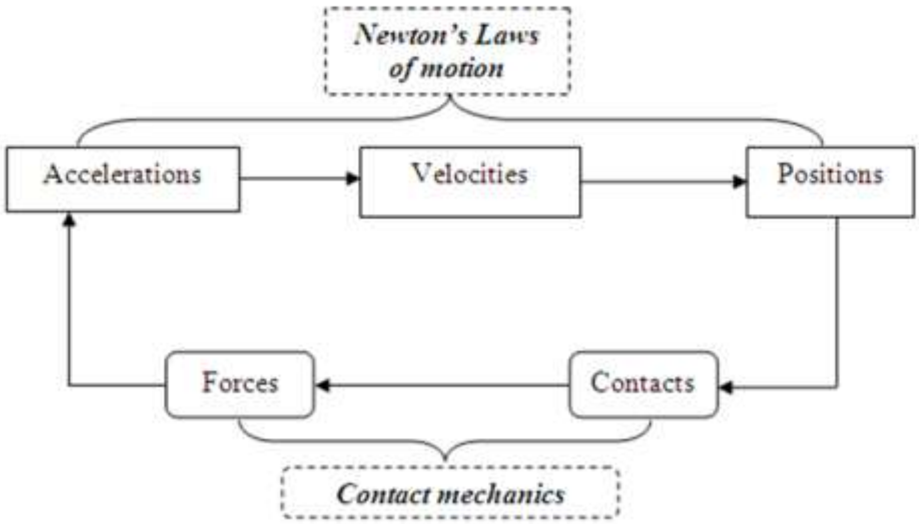
$\vec{f}_i^{\,ext}$ are external forces acting on particle i due to uniform or non-uniform external fields such as gravitational and magnetic fields.

$\vec{M}^t{}_{ij}$ represents tangential torque, produced by particle–particle collision.

$\vec{M}^r{}_{ij}$ is rolling friction

There are two primary forms of contact that can occur between particles: physical and non-physical. Physical contact denotes a state in which two particles come into direct contact, and the resultant forces from their collision adhere to established force-displacement principles. On the other hand, non-physical contact involves particles that do not make direct contact but still influence each other through various interparticle interactions, such as electrostatic or van der Waals forces [46,48].

There are three aspects of utmost importance that must be considered in the use of DEM. The first aspect is representing the individual particles under investigation. In the case of ball milling, particles are modelled as spherical in 3-D or circular in 2-D depending on the level of accuracy needed and the complexity of the system at hand. Modelling particles in 2-D simplifies the computational process because only x- and y-coordinates are then considered [41, 28]. The second aspect is inter-particle collision events. Interparticle collisions can be modelled using the hard or soft-sphere approach. In the hard-sphere approach, interaction forces are assumed to be impulsive so that particles exchange only momentum through collision. Although in the soft-sphere approach, particles are also assumed rigid, small overlaps are allowed to represent deformations during contact [46]. The last aspect is the DEM computational cycle depicted in Fig. 1. This involves the estimation of accelerations, velocities, and positions of particles. Once contact forces have been determined (bottom part of Fig. 1) using contact mechanics, particle accelerations are computed by numerical integration of Newton's laws of motion (top part of Fig. 1). In ball milling systems, the laws of motion are applied to individual balls. Each ball is treated as a separate entity experiencing combined translation and rotation. When the positions have been determined, the cycle starts over again with contact detection at the next step.



Particle collision forces

Numerous theories have been proposed to model particle collision in DEM. These models include the linear spring-dashpot system, the classical Hertz's theory for the normal direction and models developed by [39]. However, there are still grey areas about the simulation capabilities and suitability of the contact models for diverse DEM applications [55]. A step-by-step description of the collision and the dynamics of the process are discussed by [46] and [48].

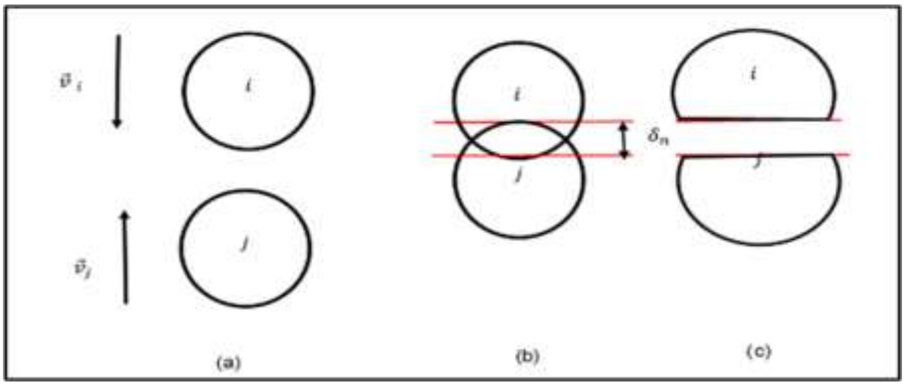
Contact forces between the colliding particles can be described using the Hertzian model as shown in Fig. 2. In this model, the contact force generated by the impact of two colliding particles is approximated to be generated along the straight line passing through the point of contact and the centres of the particles [47]. This model assumes that when two spherical particles collide, they deform by a distance δ_n (see Fig. 2 (c)). The contact force acting on particle i can then be expressed as follows:

$$m_i \frac{d\vec{v_i}}{dt} = \overrightarrow{F_{ti}} + m_i\,\vec{g} \quad 3$$

$$\vec{F}_{ti} = -q{\delta_n}^{0.25}\frac{d\delta_n}{dt} - k{\delta_n}^{1.5} \quad 4$$

In Equation **Error! Reference source not found.**) m_i is the mass of particle; $\vec{v}_i$ the velocity of particle, g acceleration due to gravity, q is the damping coefficient, k is spring coefficient, and δ_n deformation of the particle [37]. The Hertzian model offers a straightforward implementation in Discrete Element Method analysis due to its compatibility with both numerical and analytical solutions. By employing the Hertzian model, researchers and engineers can readily incorporate the necessary equations and algorithms into DEM simulations. The model's simplicity allows for efficient numerical computations, making it an accessible choice for analyzing particle interactions in granular materials.

Fig. 1. Particle contacts and overlap (a) particles approaching, (b) particle collide and overlap (c) deformed particle on contact.



The simplest and most common contact model is known as the linear spring-dashpot or LSD shown in Fig. 3 [20,14,32]. This model comprises of springs and dashpots arranged in parallel. Inclusion of springs and dashpots allows for modelling of both the elastic and viscous behaviors of the colliding particles. In the LSD model the collision force in the normal direction is defined by Equation **Error! Reference source not found.** and consists of the elastic.

$$\vec{f_{ij}}^{\,n} = \vec{f_{el}}^{\,n} + \vec{f_{diss}}^{\,n} \quad 5$$

The normal elastic force ($\vec{f}_{el}^{\,n}$) conserves the kinetic energy during collision. It is related to the normal overlap (δ_n) by the proportionality factor of spring stiffness (k_n) as illustratd in Equation 6

$$\vec{f_{el}}^{\,n} = -(k_n\delta_n)\vec{n}_{ij} \quad 6$$

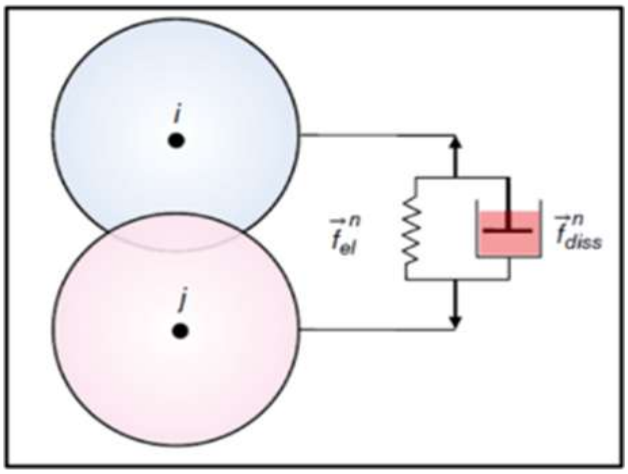
$$\vec{f_{diss}}^{\,n} = -(\eta_n v_{rn})\vec{n}_{ij} \quad 7$$

$$v_{rn} = \vec{v}_{ij}\vec{n}_{ij} \quad 8$$

Where k_n is the normal spring stiffness of linear spring.
η_n is the normal linear velocity damping coefficient.
v_{rn} is the relative velocity in normal direction.

On the other hand, the viscous force, ($\vec{f}_{diss}^{\,n}$), is proportional to the relative velocity of particles (ν_{rn}), as shown in Equation **Error! Reference source not found.**. This viscous force component disperses the kinetic energy of collision.

Fig. 2. Visco elastic model in normal direction [46]



Accordingly, the collision force in the normal direction can be approximated by

$$\vec{f}_{ij}^{\ n} = -(k_n\delta_n)\vec{n}_{ij} - (\eta_n v_{rn})\vec{n}_{ij} \qquad 9$$

[20, 37] used the LSD model of contact forces and computed particle accelerations from momentum balances. They were able to show that the normal force (F_n) can be expressed as a function of spatial overlap (δ_n) and normal relative velocity at the contact point (v_{rn}) as follows

$$F_n = -k_n\delta_n + c_n v_{rn} \qquad 10$$

When there is no tangential displacement Equation **Error! Reference source not found.**is reduced to Equation 11 below. In other words, the system is simply and better described by a non-linear relation [19].

$$F_n = -k_n\delta_n^{\ 3/2} \qquad 12$$

The tangential contact force was defined in terms of the relative tangential velocities of particles in contact. The magnitude of this tangential force is determined by the relative tangential velocities and by the Coulomb frictional limit, which is the point where the particles begin to slide over each other. The magnitude of this force is calculated as shown below:

$$F_t = min\left\{\left|k_t \int_{t_{c,0}}^{t} \delta_t dt + c_t\delta_t\right|,\ \ \mu_c F_n\right\} \qquad 13$$

Where k_t is the tangential spring coefficients, c_t the tangential damping coefficient, $\delta_t$is the tangential overlap.

In Equation**Error! Reference source not found.**, the integral term represents a spring that stores energy from the relative tangential motion which denotes the elastic tangential deformation that occurred when particles touched since time $t = t_{c,0}$.The second part, characterizes the dashpot and accounts for the energy dissipation of the tangential contact. The values of the normal and tangential spring and damping coefficients i.e. $k_{n,}$ k_t, c_n, c_t can be expressed as a function of the overlap and are discussed by[19, 48].

The total force acting on a particle can be represented as follows [31].

$$ma = \sum F_p = F_n + F_t + F_f + F_b \qquad 14$$

Where F_p are the different forces acting on the particle that include normal, tangential.

F_b is the sum of the body forces like gravity, electrostatic or magnetic acting on the particle.

F_f is the force that the fluid phase exerts on the particles.

An important benefit of employing the LSD (Linear Spring-Dashpot) model is its simplicity, which enables its analytical solution. This advantageous characteristic facilitates the straightforward implementation of the LSD model into a numerical code once the collision parameters have been estimated [46]. The simplicity of the LSD model, however, imposes limitations on the level of detail that can be obtained from the analysis of contact events. It is crucial to recognize that the idealized nature of the contact model restricts the ability to perform a comprehensive analysis of the contact event. Therefore, it is important to exercise caution and avoid over-interpreting the outputs of the LSD model in terms of their physical significance [58]. Despite these limitations, the analytical solvability of the LSD model remains a significant advantage. This feature allows for efficient implementation within numerical codes, facilitating simulations and providing valuable insights into the behavior of granular materials. While the LSD model may not capture the full complexity of contact events, it still serves as a valuable tool for understanding macroscopic behavior and obtaining approximate results.

DEM Input Parameters

Selecting and fine-tuning input parameters that accurately reflect the characteristics of particles stands out as a critical challenge in implementing the Discrete Element Method (DEM). When configuring a DEM simulation, it is imperative to establish key parameters. These critical factors encompass material contact properties (such as Young's modulus, coefficient of restitution, and coefficient of friction), the time step, and the contact model utilized.

Young's modulus (E) represents the ratio of stress below the material's proportional limit to the corresponding strain, defining the rigidity or stiffness of a material and often referred to as the elastic modulus. A particle composed of a material with a high Young's modulus exhibits minimal deformation upon collision [57]. Within DEM simulations, Young's modulus is crucial for calculating elastic deflections. While Young's modulus does not influence the final shape of the material under examination, adjusting its value significantly impacts computational time. Decreasing the Young's modulus accelerates simulations efficiently without affecting the flow behavior, leading to a common practice of artificially reducing Young's modulus to minimize simulation durations [59]. Although Young's modulus is a pivotal parameter in DEM modeling, there is a notable absence of published studies regarding its effects on the load behavior of ball mills.

The coefficient of restitution (e_n) is an indication of the residual kinetic energy after a collision of two objects [25] . A high coefficient of restitution**,** implies very little kinetic energy was lost during the collision. The coefficient of restitution can be expressed by Equation 15

$$e_n = -\frac{v_{rn,rb}}{v_{rn,imp}} = e^{-\varphi t_{col}} \qquad 15$$

In DEM, the coefficient of restitution is used to determine the normal damping coefficient (c_n). The coefficient of restitution has also been found to have a bearing on milling simulations due to small impact velocities with a strong elastic response [8]. It is still unclear how it affects the wet mill load behaviour.

Generally, particle-particle and particle-wall interactions entail contact forces both in the normal and tangential directions. However, concordant studies have highlighted the significance of rotational inertia and energy loss in rotation of particles [3,4]. These should be accounted for when modelling dynamic granular systems such as ball mills. One way of doing that is to describe the frictional forces acting on particles: the rolling and sliding frictions. The two types of friction cause resistance to rolling and sliding respectively. They are defined as follows [3]:

$$F_r = \mu_r F_n \qquad 16$$

Where μ_r is the coefficient of rolling friction for the two surfaces in contact.

F_r is the resistive force of rolling friction

F_n is the normal or perpendicular force of the particle on a surface

When a torque is applied to a stationary mill, static rolling friction holds back the motion of the charge. As the mill rotates, a point is reached when the load begins to slide down the mill. At this point, the sliding friction starts to act on the load. This is captured by the coefficient of sliding friction [3].

$$\mu_s = \frac{F_s}{F_n} \qquad 17$$

Where μ_s is the coefficient of sliding friction for the two surfaces in contact

F_s is the resistive force of sliding friction

F_n is the normal or perpendicular force of the particle on a surface

The coefficient of sliding friction (μ_s) is a dimensionless number that indicates the amount of sliding friction between two objects for a given normal force Equation **Error! Reference source not found.**. In DEM modelling, the effects of friction can be determined by varying both the coefficient of rolling friction and the coefficient of sliding friction.

Choosing a suitable time step is an important process. Particle movement in dense multiphase systems is not only affected by neighbouring particles but also by distant particles. The general approach is to choose a numerical time step less than a critical value with the view to allowing the disturbance to propagate between immediate neighbouring particles only [16]. Two methods can be used to determine the critical time step size: the Rayleigh and the Hertz methods. For a particle (i) the Rayleigh time step is given by [33]

$$t_R = \frac{\pi r_i}{(0.1631\nu_i + 0.8766)}\sqrt{\frac{\rho_i}{G_i}} \quad 18$$

Where G_i is the shear modulus of the particle given by

$$G_i = \frac{Y_i}{2(\nu_i + 1)} \quad 19$$

Here, ν_i is the Poisson's ratio and Y_i is the Young's modulus of the particle. The Rayleigh time step solely depends on the particle properties, and thus will remain constant during the simulation for a given set of particle properties [33, 34]. The Hertz time step is given by

$$t_{Hertz} = 2.87\left[\frac{{m_{eq}}^2}{r_{eq}{Y_{eq}}^2 v_{max}}\right]^{0.2} \quad 20$$

Where m_{eq}, r_{eq}, Y_{eq} are the equivalent mass and radius of the particle and its Young's modulus respectively. And ν_{max} is the magnitude of the maximum relative velocity between the particles.

The choice of time step is a trade-off between the accuracy of the model and computational time. Generally, for dense multiphase systems, a time step between 15 and 30 % of critical time is acceptable, and gives results that are close enough for industrial applications [34]. Equation **Error! Reference source not found.** shows that increasing Young's modulus of the particle results in a corresponding increase in time step. Hence, a frequently used technique to increase the time step while reducing computational time is to lower the particle stiffness.

The computational procedure for DEM simulations can be summarized as follows: The first step is the simulation setup in which particle data, geometry, and properties of particles and walls are read into the program. This is followed by an initialization process that includes defining all initial position and velocity vectors, particle and wall properties that are required to compute contact forces. The second step is launching of the particle iteration loop which controls the insertion of particles. The third step is the prediction of position and velocities of particles at the next time step, using the history of position, velocity, and acceleration of particles. It is at this stage that all contact forces are computed using the contact model [46, 32].

Last note, a DEM simulation algorithm must allow predictable translations and rotations of the discrete bodies, recognize new particle-particle interactions, and allow complete detachment during the computation process. In the literature, early applications of the DEM in modeling comminution in ball mills predominantly concentrated on simulating the motion and interactions of the grinding media, often overlooking the significant influence of the slurry dynamics on the overall milling process.[Larsson] DEM techniques become inadequate for multiphase granular systems composed of more than one phase. Wet milling is one such a system consisting of two phases: the solid phase made up of grinding balls and the liquid phase or slurry. DEM can only model the solid phase of a wet mill while the liquid is dealt with using a different computational framework described in the next section.

Computational modelling of the liquid phase in multiphase granular systems

Work done by [1,11,13,18,40,50,51] demonstrate that DEM can be successfully used in dry mill modelling. To simulate wet milling, better knowledge of the flowing fluid and the position of slurry with respect to media charge are required. A technique known as Computational Fluid Dynamics (CFD) is used to this end. Physical aspects of flowing fluid can be described by three governing principles. These are conservation of mass, Newton's second law, and energy conservation. Often-times, these expressions are in the form of integral or partial differential equations depending on the flow models from which they are derived. The CFD framework replaces the integrals or derivatives in the differential equations with discretized algebraic forms. These new expressions are solved to obtain numbers of the flow field values at discrete points in space and time.

CFD Computational Fluid Dynamics (CFD) methods are broadly classified into two main categories: Eulerian and Lagrangian. This classification is based on the different perspectives that Leonhard Euler and Joseph-Louis Lagrange held when observing fluid flow [53].

The Eulerian approach focuses on specific locations in the space through which the fluid flows as time passes. This means the computational grid is fixed, enabling the solver to calculate the velocity at each grid point. Widely used Eulerian methods include the Finite Difference Method (FDM), Finite Volume Method (FVM), and Finite Element Method (FEM).

In contrast, Lagrangian methods do not use a fixed mesh, but rather track individual fluid particles that can move freely through space. This allows the observer to follow the motion of individual fluid particles as they move through space and time. One of the most widely used Lagrangian methods is Smoothed Particle Hydrodynamics (SPH).

To describe complex multiphase granular systems, researchers have developed hybrid CFD-DEM (Discrete Element Method) models that combine Eulerian and Lagrangian approaches. These hybrid models can capture the interactions between the fluid and solid phases more accurately [15,54,6,35,56,27,37].

Modelling the liquid phase in multiphase granular systems

The general approach to modelling the flow of the fluid phase in a multiphase system is based on solving the Navier-Stokes and continuity equations [15,37, 20,35]. The continuity and the Navier-Stokes equations can be represented in their generic form by Equation (2.58) and Equation (2.59) respectively [26,46].

$$\frac{\partial \alpha_f}{\partial t} + \nabla\left(\alpha_f u_f\right) = 0 \qquad 21$$

$$\frac{\partial(\rho_f\, \alpha_f\, u_f)}{\partial t} + \nabla\left(\rho_f \alpha_f u_f\right) = \nabla\rho - f_p + \nabla.\left(\alpha_f \tau\right) + \rho_f \alpha_f g \qquad 22$$

Where α_f is the volume fraction occupied by the fluid, ρ_f is the fluid density, u_f velocity of the fluid, τ is the stress tensor for the fluid phase and f_p represents the momentum exchange with the particulate phase. When both the granular and fluid phases are incompressible, [37] showed that the mass conservation equation could be written as follows

$$\nabla.\left(\alpha_f u_f + \alpha_s u_s\right) = 0 \qquad 23$$

Where α_s is the volume fraction occupied by the solid phase, u_s velocity of the solid phase.

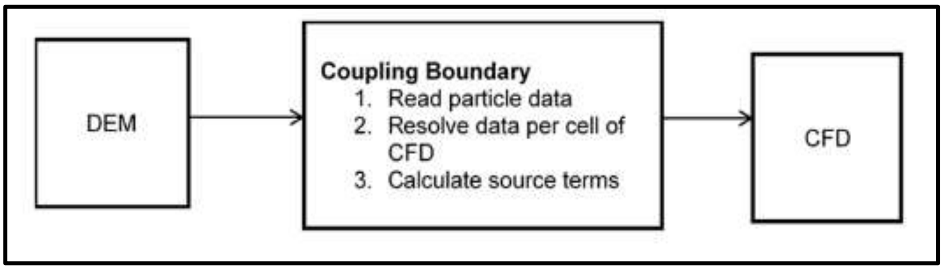
When a solid particle moves through a fluid, the fluid and surrounding particles exert a force against the particle called drag force. The magnitude of the drag force depends on the slip velocity between the fluid and the solid as well as the porosity of the system amongst others. A portion of the drag force may also emanate from the surrounding solids present in the fluid. In order to estimate this contribution, the solid fraction (α_s) and the solid field velocity (u_s) are computed from the DEM simulations. This provides initial information on the forces exerted on the particle under consideration for the estimation of the drag force. The drag force can then be obtained by integrating the stress tensor over the particle surface.

Interactions Coupling in multiphase granular systems

Multiphase granular systems can be modelled by combining DEM and CFD methods in a suitable framework. Generally, this is done by applying the DEM to the solid phase and the CFD to model the flow patterns of the liquid phase. The DEM and CFD solvers are allowed to exchange data in process called coupling [31,21, 37,54,6,35,56]. The coupling concept is used to describe interactions between liquid and solid phases. It occurs through the exchange of momentum and interaction forces between phases. The fluid phase is described by defining the distributions of pressure, velocity, temperature, and species concentration in the flow field. The solid phase, on the other hand, is described by size, position, velocities, temperature, and concentration. This approach is novel in that it allows for the solution of solid particle-particle interactions, fluid flow field, and particle-fluid interaction equations [32,37,46].

The principal steps for DEM-CFD coupling have been extensively discussed by [20] and [31]. The coupling routine consists of first calculating the positions and velocities of solid particles using a DEM solver. Then, the computed results are passed to the CFD solver. Corresponding cells are determined in the CFD mesh for particles; then, the volume fraction and average velocity of particles are determined. From here, the computation of fluid forces acting on particles based on the particle volume fraction is done. The last step is to determine particle-fluid momentum exchange by collectively averaging all particle-fluid forces acting on each particle in a CFD cell. When these steps are completed, the calculated data is sent to the DEM solver and used within the next time step. The CFD solver outputs the fluid velocity considering local volume fraction and momentum exchange. The key steps of DEM-CFD coupling are as shown in Fig 5.

Fig. 3. Coupling Interface [37]



The suitability of a multi-physics model to replicate a physical multiphase system will be a function of the chosen coupling strategy. Interactions between phases can be grouped into four classes ranging from one-way to four-way coupling. In order to determine the appropriate coupling strategy for a system, the type of interphase transfer between phases, the mutual interactions of fluid and solid phases, the effect of particle concentration on the coupling must be considered.

One-way coupling describes a system in such a way that the motion of the dispersed solid phase is primarily affected by that of the continuous fluid phase. The motion of solid phase particles is assumed to have negligible influence on the motion of continuous phase. In this case, the equations of the fluid phase can be solved independently from equations of particles the Lagrangian way [46]. [44] applied one-way coupling method to a wet ball mill. The effects of slurry on the motion of individual balls were modelled by including drag and buoyancy defined by Equations **Error! Reference source not found.** and **Error! Reference source not found.**

$$F_D = C_d A \rho_s \frac{{v_r}^2}{2} \qquad 23$$

Where F_D is the drag force.

C_d is the drag coefficient.

A is the area of grinding media.

v_r is the relative velocity between a ball and suspension.

The buoyant force, on the other hand, was given by

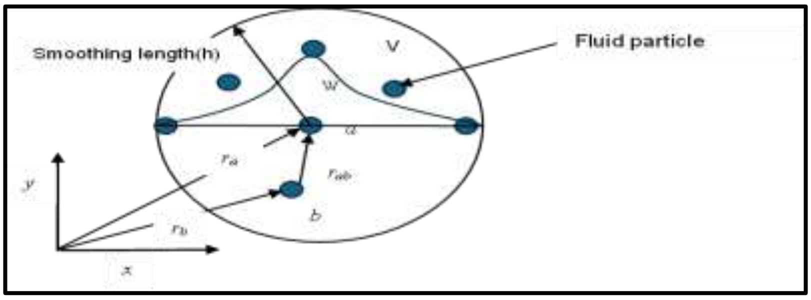
$$F_B = V_B \rho_s \qquad 23$$

Where F_B is the buoyant force and V_B is the volume of a ball

Slurry was assumed to be horizontal and undisturbed. Upon identifying and locating balls below the slurry level, drag and buoyancy were applied to them in addition to other forces. In doing so, wet milling was studied using the modified DEM algorithm that a has concept of the buoyancy and viscosity of the slurry in a mill. Although useful information was extracted, the assumption that the slurry was horizontal was an oversimplification of the load behaviour of a real mill. Concordant research has shown that the profile of the load is crescent-shaped following the direction of rotation of the mill [29]. Furthermore, the study does not simulate the slurry flow in the mill. As such, the proposed one-way coupling model may be regarded as inadequate since the slurry position is not stagnant.

Smoothed Particle Hydrodynamics (SPH) is a mesh-free computational procedure used for simulating the mechanics of continuum media such as fluid flow. This method works by dividing the fluid into a set of discrete elements, referred to as particles. These particles have a spatial distance (known as the "smoothing length represented by h in Fig. 6), over which their properties are "smoothed" by a kernel function. These particles represent an interpolation grid that is used to compute the fluid properties at any given point in the simulation domain by using an interpolation function called the ‘Kernel’ [53].

Fig. 4 Illustration SPH[43].



$$A(r) = \int A(r')W(r - r', h)\, dr \qquad 24$$

The interpolated value of a function A at any position r can be expressed using SPH smoothing as shown in equation 30

$$A_s(r) = \sum_b m_b \frac{A_b}{\rho_b} W(r - r_b, h) \qquad 25$$

Where the summation index b denotes a particle label, and the summation is over all particles b within a radius 2h of r. Particle b has mass m_b, position r_b, density ρ_b, and velocity v_b The value of any quantity A at r_b is denoted by A_b [43].

Recently, [12] approached the wet milling problem by applying one-way coupling to DEM and Smoothed Particle Hydrodynamics (SPH)Coupling was performed by simulating grinding media flow in LIGGGHTS, then the data describing the velocity field was transferred to SPHysics. Finally, the slurry flow field was estimated from SPHysics. In all the DEM-SPH simulations presented by [12], the slurry appears to be stagnant (like [44]. One would expect this to be acceptable at low mill speeds but not at speed above, say, 60 % of critical. Furthermore, no pool position information was presented in the study.

Two prominent proposals for one-way coupling have been reviewed: [44], as well as [12]. In both cases, the coupling assumed that the motion of grinding balls does not affect that of the slurry. The slurry was assumed stationary and only allowed to create drag and buoyancy around immersed balls. This simplification basically forced the slurry not to percolate through the dynamic bed of balls. The shortcoming is partially addressed with two-way coupling schemes.

It is widely accepted that the motion of particles affects the motion of fluid phase in a wet ball mill and vice versa. When modelling is done by replicating the bidirectional interaction, the flow is said to be two-way coupled. Particle-induced fluid disturbances such as wakes behind a particle are a typical example of two-way coupling [7].

[15] coupled DEM and Smoothed Particle Hydrodynamics (SPH) to predict the slurry flow patterns within an SAG mill. In their work, the DEM was used to describe the motion and interactions of individual balls which formed a bed of heterogeneous porosity. The SPH was employed to model the slurry as a fluid of given rheological properties. Cleary et al. (2016) presented the media charge as a dynamic porous bed through which the SPH fluid can flow. They were able to combine the two concepts under what is called "DEM-SPH framework" to allow for the interaction between the two systems. The porous media is characterized by the solid fraction and velocity distributions calculated from the DEM simulation. The coupling of the slurry to the porous media is accomplished by applying the Darcy law drag which is suitable for modelling porous media [15].

$$F_{drag} = \varepsilon^2 \mu_a \left(\frac{v_a - v_{DEM}}{\rho_a K_{DEM}}\right) \qquad 25$$

where ε is the porosity (void fraction) of the porous media

μ_a is the fluid viscosity for SPH fluid particle a

v_a is the velocity of SPH fluid particle a

v_{DEM} is the DEM solid velocity at that point (interpolated from the grid)

ρ_a is the fluid density of particle a

K_{DEM} is the permeability of the porous media

In doing so, they managed to describe the entire system constituting the wet mill load. The porosity of the bed as well as the motion and distribution of slurry within the load are amongst the most insightful information one can get from the DEM-SPH simulations.

However, the DEM-SPH coupling has one main drawback. Even though SPH is a powerful tool capable of handling many types of material behaviors, it is rather slow and numerically unstable under extreme fluid deformations present in wet mills. As such, there is still limited understanding on how solid media and slurry interact

In some cases, disturbances of the liquid phase in the form of eddies and wakes affect the motion of particles. This phenomenon needs to be modelled using what is called three-way coupling. In addition to interactions between solid and fluid phases, particle-particle collisions can also influence the overall motion of phases leading to a four-way coupling problem. Four-way coupling is suitable for modelling dense flows with high frequency of collisions between particles [46,60]. Understandably, this type of coupling is computationally intensive and yet to be applied to wet milling.

Programming Perspective

Numerical modeling of multiphase granular systems often involves combining Discrete Element Method (DEM) and Computational Fluid Dynamics (CFD) solvers. These coupling routines are typically offered as commercial software packages like RockyDEM and ANSYS, which can be quite costly and are generally restricted to shared memory machines [36]. To address the issue of high costs, open-source codes have been proposed as viable alternatives for DEM and CFD analysis [31,15,12]. However, these open-source codes are not fully developed and can be challenging to program. Examples of such open-source software include DEM solvers like LIGGGHTS and YADE. CFD solvers like OpenFOAM and SPHysics, the latter being particularly popular due to its programmability and adaptability, are also employed in this context. LIGGGHTS (LAMMPS Improved for General Granular and Granular Heat Transfer Simulation) is an open-source software used for modeling granular material within the DEM framework. It incorporates LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), a conventional molecular dynamics solver used to model a wide range of materials (Plimpton, 1995).

Interestingly, there appears to be no published research on the application of two-way LIGGGHTS-OpenFOAM coupling in wet ball milling. However, based on our extensive literature review, it is evident that LIGGGHTS-OpenFOAM possesses all the essential capabilities to accurately simulate the dynamics of wet ball mills

Conclusion

Understanding the behaviour of the mill load is fundamental for optimizing the efficiency of wet ball mills, which are integral to numerous industries. Numerical modelling has proven invaluable in elucidating the internal macroscopic and microscopic processes within ball mills. Among these modelling techniques, the Discrete Element Method (DEM) stands out as a powerful framework that offers intricate details on charge motion, collision forces, energy dissipation, and power consumption, among other critical parameters.

However, it's important to note that DEM is primarily tailored for dry mills, and there exists a dearth of literature concerning how material properties influence the dynamic load behavior in wet milling scenarios. To effectively model wet milling processes, a comprehensive toolkit capable of simulating media, slurry, and their complex interactions concurrently is essential.

Given the intricate nature of wet milling systems, researchers have employed various strategies, from adapting dry milling simulations and adjusting outputs for wet environments to employing simplifying assumptions specific to wet milling conditions. Computational simulations, particularly the integration of Computational Fluid Dynamics (CFD) with DEM, have revolutionized the exploration of wet ball milling by offering invaluable insights at a fraction of the cost associated with experimental testing. The utilization of CFD-DEM as a numerical approach for simulating wet ball milling has significantly propelled our comprehension of the intricate interplay among diverse factors influencing mill performance.

Future research endeavours should prioritize the refinement of drag correlation models to enhance the precision of simulating slurry behaviour within milling processes. An imperative lies in integrating intricate phenomena into computational models to elevate simulation accuracy, offering a deeper insight into wet ball milling operations. A pivotal unexplored area in wet ball mill modelling pertains to the direct inclusion of ore particle (referred to as powder in dry milling) effects in a coupled CFD-DEM model. As milling progresses, the transformation of slurry properties alongside the grinding of ore particles is anticipated. While some scholars advocate for representing the powder effect through slurry viscosity, a notable research opportunity persists in optimizing the incorporation of particle breakage in wet ball milling models, particularly regarding the impact of grinding media on the slurry flow field.

In conclusion, this paper emphasizes the importance of computational simulations in understanding and optimizing wet ball milling processes, while also highlighting the need for further research, collaboration, and comprehensive reviews to advance the field and unlock the full potential of wet ball mills in various industrial applications.

Acknowledgment
This work was financially supported by the Univeristy of South Africa

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