Heterarchical model of comminution in high pressure grinding rolls

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Abstract. High pressure grinding rolls (HPGR) are commonly used for material grinding in industries such as mineral processing, cement production, and chemical manufacturing. Comminution modelling for these devices is typically performed using either continuum-based population balance models or particle-based numerical tools such as the discrete element method (DEM). However, population balance models overlook the complex interplay of particle crushing, segregation, and mixing that occurs during comminution, limiting their effectiveness in accurately predicting device performance under varying operating conditions. Similarly, DEM models are limited by their high computational cost, which restricts their ability to track only a limited number of particles and simulate their sequential crushing. Here, we overcome the limitations of these traditional modelling approaches by exploring a novel heterarchical model for HPGR comminution. The heterarchical model captures the physics of particle crushing, segregation, and mixing while efficiently handling an arbitrarily large number of particles. Therefore, this model allows for the prediction and analysis of HPGR performance by tracking the evolving particle size distribution at any point in space and time.

1 Introduction

The high pressure grinding roll (HPGR) is a widely adopted technology in the comminution industry, offering significant advantages in grinding efficiency compared to traditional milling methods [1]. An HPGR consists of two counter-rotating rolls (see Fig. 1), one fixed and the other free to move, applying pressure to compress the material as it passes through a gap between them.

Modelling comminution in HPGR is challenging due to complex granular flow dynamics involving coupled crushing, segregation, and mixing of particles. In the existing literature, comminution in HPGR is commonly modelled using two different approaches. The first approach is based on population balance models (PBMs) [2], which use empirical breakage and selection functions to predict the performance of HPGRs in terms of particle size distribution (PSD), throughput (*i.e.,* amount of crushed material passing through rolls per unit time) and power draw. The major drawback associated with these models is that they tend to ignore the particle-based physics dictating the comminution and instead constantly end up recalibrating their in-built empirical functions whenever the operating conditions change beyond their predefined range. The second approach employs numerical tools, such as the discrete element method (DEM) [3, 4]. DEM is an excellent tool for studying HPGR comminution, offering insight into particle-scale crushing and system behaviour. However, its high computational cost makes it impractical for HPGRs, which process a vast number of particles, especially as they crush into small fragments. Besides these commonly used approaches, comminution in HPGR has also been explored using a continuum model based on breakage mechanics in [5].

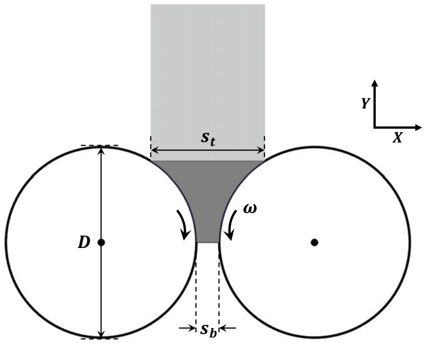

Figure 1. Schematic of high pressure grinding roll (HPGR). An HPGR consists of two counter-rotating rolls, one of which is fixed while the other can move freely. The material to be crushed is fed through the gap between these two rolls. Here, the material being fed is shown in *light grey* while the material that is undergoing compression is shown in *dark grey*. In the paper, only the material in *dark grey* is modelled.

To provide an alternative perspective on comminution modelling and address certain limitations of existing approaches, a multiscale modelling approach based on the novel concepts of heterarchy [6] has been proposed in [7–9] for comminution in rotary mills. The heterarchical model, unlike PBMs, can explain the detailed physics governing the comminution in HPGRs, without ignoring particle crushing, segregation, and mixing. At the same

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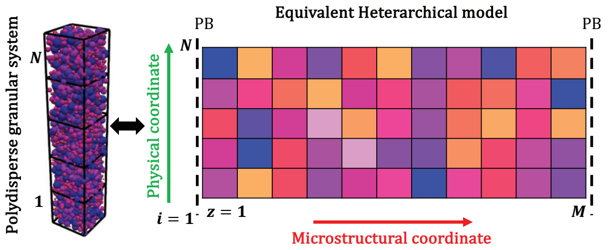


Figure 2. A physical polydisperse granular system (*left*) and its equivalent heterarchical model (*right*). The physical system is discretised into representative volume elements (RVEs). Each RVE is further discretised along the internal microstructural coordinate into M cells with periodic boundary (PB) conditions [7].

time, unlike DEM models, it can accommodate an arbitrarily large number of particles without excessive computational costs.

In this study, we apply the heterarchical modelling approach for comminution in HPGR. To achieve this, we incorporate continuum granular elasticity to estimate the stress field in the material between the rolls, which governs the crushing process. We present preliminary results from this model, focusing on the pressure profile within HPGR and the resulting product particle size distribution (PSD).

2 Heterarchical model for comminution

This section provides a brief outline of the fundamental heterarchical modelling and the underlying physics governing particle crushing, segregation, and mixing. The section next moves on to discuss its extension to model comminution in HPGRs.

2.1 Basic framework

In the original heterarchical framework proposed in [6], a system of polydisperse particles is discretised into representative volume elements (RVEs) along the physical spatial coordinates, as shown in Fig. 2. Each RVE is further subdivided along an internal microstructural coordinate, where particles within the RVE are mapped into discrete cells. The position of these cells along the microstructural coordinate represents the local neighbourhood of particles. This transformation replaces the real particle system with an equivalent stochastic lattice, where each cell contains particles of a specific size.

To model particle crushing, segregation, and mixing within the stochastic lattice, the heterarchical framework defines a set of rules governing these mechanisms. The crushing rule dictates that for each cell along the microstructural coordinate within a given RVE, the external stress acting on the particles is compared to their crushing strength. If the external stress exceeds the crushing strength, the particle size in that cell is reduced by a certain factor, otherwise, it remains unchanged. For segregation and mixing, which involve the movement of particles in physical space, the heterarchical rule is such that the particles in a given cell are swapped with their neighbouring cells at a certain frequency. In the case of segregation, which here arises due to differences in particle size (among other factors), this frequency is a function of neighbouring particle size. In contrast, mixing results from random fluctuations during flow, and is therefore random, making it independent of the neighbouring particle size.

2.2 Application to high pressure grinding rolls

The heterarchical physics of particle crushing, segregation, and mixing within HPGR is implemented by integrating these grainsize dynamics along the streamlines of the granular flow. To define the streamlines, we first assume a symmetric flow on either side of an axis passing through the midpoint of the gap. The streamlines are then represented as a cubic polynomial, bounded by the roller edges and the central line of the gap, as illustrated in Fig. 3a.

Next, we prescribe a velocity distribution for particles within the gap. At this stage, we adopt a simple velocity distribution, with particle velocity ranging from zero ($v = 0$) at the top of the flow to a value equal to rotational velocity ($v = \omega r$) at the bottom, as shown in Fig. 3b. This approximation is reasonable, as it aligns with velocity distributions obtained from DEM simulations [10]. However, in the future, a more refined velocity model can be developed.

With both velocity field and streamlines defined, we next discretise each of the streamlines into a set of material points by marching along the streamline length in discrete time steps as shown in Fig. 3c. The volume occupied by these material points is determined using Voronoi tessellation as shown in Fig. 3d.

The crushing mechanism is implemented using the following criterion [7] for the onset of particle breakage

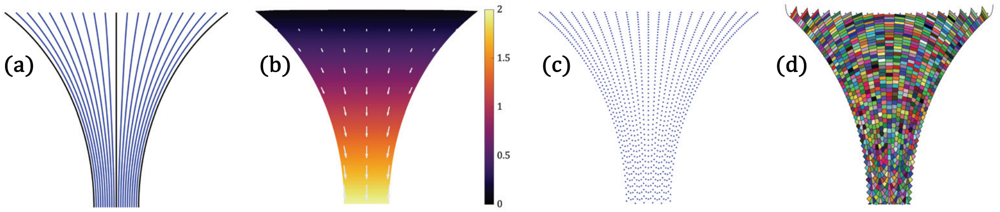
$$s^{t+\Delta t}_{i,j,p} = \begin{cases} X^t_{i,j,p} s^t_{i,j,p} & \text{if } \sigma_a \cdot \mathcal{H}(\dot{\varepsilon}_v) \geq \sigma^{s^t}_{i,j,p}(s) \\ s^t_{i,j,p} & \text{otherwise,} \end{cases} \tag{1}$$

where i, j are the spatial coordinates, p is the microstructural coordinate, $s_{i,j,p}$ is the particle size in the cell (i, j, p), $X_{i,j,p}$ is the reduction factor between 0 and 1 drawn from a fragment size distribution, σ_a is the external stress, $\dot{\varepsilon}_v$ is the volumetric strain rate, and $\mathcal{H}$ is the Heaviside function. The crushing strength $\sigma^s_{i,j,p}$ of the particles in cell (i, j, p) is given as [7]

$$\sigma^s_{i,j,p}(s) = \sigma^m \left(\frac{s_{i,j,p}}{s^m}\right)^{-3/w_s} \exp\left[\frac{\log^2(s_{i,j,p}/\bar{s}_{i,j,p})}{2n^2}\right], \tag{2}$$

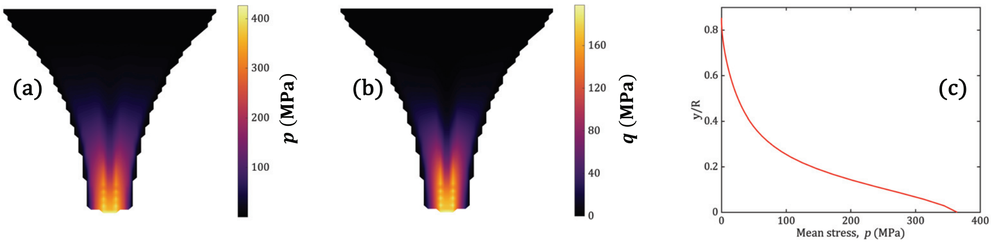
where σ_m is the crushing strength of the maximum particle size s_m, w_s is the Weibull modulus, $\bar{s}_{i,j,p}$ is the average particle size considering particles in cell (i, j, p) and its immediate neighbours, and n is a scaling constant.

The segregation and mixing mechanisms are implemented by swapping of particles of size (s) in the cell (i, j)



Streamlines for the granular flow | Velocity field (magnitude only) | Material point distribution along streamlines | Volume of material point using Voronoi tessellation

Figure 3. Application of heterarchy in high pressure grinding rolls (HPGR): (a) Streamlines for the granular flow, (b) Velocity field, (c) Material point distribution along the streamlines using a timestep (Δt), and (d) Volume corresponding to each material point determined using Voronoi tessellation.



Mean stress (p) | Triaxial shear stress (q) | Mean stress (p) variation along depth

Figure 4. Particle stresses within high pressure grinding roll (HPGR) obtained using continuum granular elasticity: (a) Mean stress (p), (b) Triaxial shear stress (q), and (c) Mean stress variation along depth measured at the centre of roller gap.

along the neighbouring cell (q) with a frequency $f^{swap}_{i,j,s,q}$, given as [8]

$$f^{swap}_{i,j,s,q} = \frac{l_{ijq}}{\rho_b V_{ij}}(\vec{F}_{i,j,s} \cdot \hat{n}_{ijq}), \qquad (3)$$

where l_{ijq} is the length of the Voronoi edge along the q^{th} neighbour, ρ_b is the bulk density, V_{ij} is the volume of cell (i, j), $\vec{F}_{i,j,s}$ is the material mass flux due to advection and diffusion, and $\hat{n}_{ijq}$ is the unit normal vector to the Voronoi edge q for cell (i, j).

To estimate the applied stresses on particles during the 'compacting flow' in HPGR, we use continuum granular elasticity [11, 12] as a simple constitutive relation for the stress rates

$$\begin{bmatrix} \dot{p} \\ \dot{q} \end{bmatrix} = 3\overline{G}\phi^3\varepsilon_v^c \begin{bmatrix} \frac{\overline{K}}{3\overline{G}} + \frac{c(c-1)}{2}\eta^2 & c\eta \\ c\eta & 1 \end{bmatrix} \cdot \begin{bmatrix} \dot{\varepsilon}_v \\ \dot{\varepsilon}_s \end{bmatrix} \qquad (4)$$

where $\dot{p}$ and $\dot{q}$ are the triaxial mean stress rate and triaxial shear stress rate, $\overline{K}$ and $\overline{G}$ are scaling parameters for the bulk and shear moduli, ϕ is the solid fraction, $\dot{\varepsilon}_v$ and $\dot{\varepsilon}_s$ are the volumetric and triaxial shear strain rates, c is constant controlling pressure-sensitivity, and η is the ratio of volumetric to triaxial shear strain. Most simply, using very small time steps Δt the stress rates can be integrated using Euler integration along the streamlines to obtain particle stresses: $p^{t+\Delta t} = p^t + \dot{p}\Delta t$ and $q^{t+\Delta t} = q^t + \dot{q}\Delta t$.

3 Preliminary results

In this section, we present preliminary results from the heterarchical comminution model for HPGR, incorporating stresses estimated through continuum granular elasticity.

For simulation, we use the HPGR dimension as used in [10], with roller diameter $D = 6$ m, roller gap at top $s_t = 1140$ mm and bottom $s_b = 60$ mm, and roller speed of $\omega = 19$ rpm. The feed consists of particles of uniform size distribution between 8 mm and 60 mm. The feed material is chosen as quartz with elastic constants taken as $\overline{K} = 28.3$ MPa and $\overline{G} = 13.1$ MPa corresponding to Fontainebleau sand [13]. The crushing strength parameters $\sigma_m = 0.84$ MPa for $s_m = 60$ mm and $w = 3.04$ for quartz are estimated from [14].

In HPGRs, both experimental studies [15] and numerical simulations [3, 4] have shown that particle stresses increase rapidly as the roll gap decreases, reaching a maximum at the point of minimum gap. As a result, the high pressure region, commonly referred to as the grinding zone (located between the start of the nip angle and the point of minimum gap [16]), is where particle crushing primarily occurs. Additionally, stress varies along the gap, gradually increasing from the roller end, peaking at the midpoint, and then decreasing towards the other roller end. Using continuum granular elasticity, we observe a similar stress distribution within the HPGR. As shown in Figs. 4a-c, particle stress rises sharply with depth and follows a similar variation along the gap, consistent with experimental and numerical observations.

Using the heterarchical model, we further investigate comminution in HPGR. The physics rules dictating the particle crushing, segregation, and mixing are implemented as described in Sec. 2.1. As shown in Fig. 5, we measure the cumulative distribution function (CDF) of the product particle size coming out of the HPGR at different locations along the gap width (*i.e.,* along x-direction, see Fig. 1). We see a much finer product coming out through the centre of the gap width as compared to the product coming through the ends (*i.e.,* close to roller ends). It has been measured experimentally [17, 18] that the product size varies along the gap, with the fineness of the product increasing from the end to the centre and then decreasing to the other end. The heterarchical model allows us to measure the full PSD and its evolution with time.

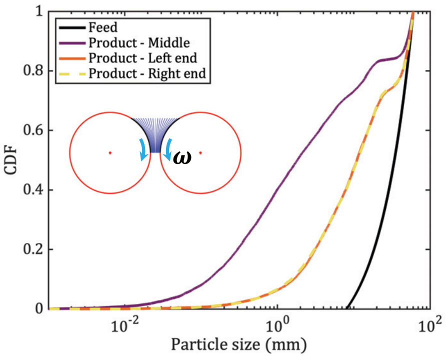


Figure 5. Cumulative distribution function (CDF) of product particle sizes at different locations along the roller gap width.

4 Conclusions

This study has presented a methodology for modelling comminution in high pressure grinding rolls (HPGRs) using a novel heterarchical model coupled with continuum granular elasticity. The model explains the comminution in HPGRs by coupling the mechanisms of particle crushing, segregation, and mixing, while being able to accommodate an arbitrarily large number of particles. Preliminary results demonstrate that continuum granular elasticity gives a realistic stress profile within the HPGR, and the heterarchical model enables prediction of particle size distributions at any given point in space and time.

In future work, this model can be used to assess the performance of HPGRs in terms of the pressure variation with roller gap, fineness of product particle size, and throughput (the rate of crushed material exiting the roller).

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