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Original Research Paper

A discrete element method-based approach to predict the breakage of coal

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ABSTRACT

Pulverization is an essential pre-combustion technique employed for solid fuels, such as coal, to reduce particle sizes. Smaller particles ensure rapid and complete combustion, leading to low carbon emissions. Traditionally, the resulting particle size distributions from pulverizers have been determined by empirical or semi-empirical approaches that rely on extensive data gathered over several decades during operations or experiments, with limited predictive capabilities for new coals and processes. This work presents a Discrete Element Method (DEM)-based computational approach to model coal particle breakage with experimentally characterized coal physical properties. The effect of select operating parameters on the breakage behavior of coal particles is also examined.

1. Introduction

The comminution process has wide applications in several industries, including mining, power, cement, paint and pharmaceuticals. The design and operating conditions for comminution devices traditionally have been determined by empirical or semi-empirical approaches derived from the vast data gathered over the years during operations or experiments. Most of these process models are based on the Population Balance Method (PBM) [5,6,19]. Some recent applications of PBM approaches in milling processes are given in [9,32,43]. A comprehensive review on the fundamental bases of the PBM and its use for varied applications is provided in [33].

One of the major applications of comminution in the power industry involves the pulverization of coal to attain rapid and complete combustion. In a coal-fired power plant, raw coal is pulverized and partially dried in a mill prior to combustion. The pulverized coal is then carried to the combustion chamber by fluidizing the coal particles using pre-heated air. The size distribution and shape of the coal particles have a significant impact on the efficiency of the mill and combustion process (also noted in [54]). Computational models for coal combustion also rely on the input coal particles distribution after the pulverization process [17,36].

The design of these mills traditionally has been based on the process models [35,42], which rely on the breakage distribution of coal derived from Population Balance approaches. The Population Balance Models are typically developed for particular devices operating in a specific scenario. However, the breakage behavior depends on the intrinsic physical properties of the coal. The PBM derived for one particular coal might not be suitable for a different coal type. Also, if there are changes in the pulverizer design or operating conditions, these phenomenological models will require further tuning. With the ever-increasing need for accuracy and sophistication in the predictive capability of comminution models, the importance of mechanistically driven computational models is growing.

The Discrete Element Method (DEM) [16] provides an alternative mechanism-based modeling capability in understanding the breakage behavior of granular material. It has been extensively used in several applications to model fragmentation and breakage of granular materials. A comprehensive review regarding the contributions of DEM for modeling comminution process is provided in [52]. Today, there are several commercial and open-source DEM software programs available. A summary of the capabilities of some of these softwares, with an emphasis on modeling techniques for fracturing processes, is provided in [22]. Many researchers [18,21,41,48] use hybrid techniques where DEM is used in conjunction with PBM. Such techniques typically consist of either

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Nomenclature

Symbols

F_n	normal interaction force between particles
K_n	normal interaction stiffness
k_n	individual particle stiffness
E	particle-scale modulus of elasticity
u_{eq}	equilibrium distance between particles
k_s	shear interaction tangent stiffness
ν	particle-scale Poisson's ratio
k_r	rotational stiffness
σ_c	normal cohesion parameter
ϕ	internal friction angle
τ_c	shear cohesion parameter
γ_{int}	interaction ratio
ΔT_{cr}	critical time step size
ρ	particle-scale density

using DEM simulations to determine certain components in the PBM or using these two methods at different length scales with the transfer of information across scales.

Broadly speaking, two approaches are typically employed in modeling the dynamic breakage of granular samples using DEM. The first approach is based on the Bonded Particle Model (BPM) [30], where particles are bonded together using some mechanical constitutive laws. The breakage in this approach is controlled by the strength and mechanical properties of each bond. Examples of similar approaches from the literature include [20,39,45–47,51]. One of the biggest challenges of this approach is that it leads to a large number of particles in the simulation, making it especially difficult to use for large-scale applications. An alternative approach is the *replacement strategy* [11–13,15]. This strategy involves a rule that is used to determine the expected conditions for particle fracture and then replaces the parent particle with a closely packed assembly of daughter particles. The choice of packing and sizes of these daughter particles usually is rather arbitrary. The packing must be carefully chosen so as to not induce any artificial stresses, which leads to a loss of mass in the system. This approach also requires particle crushing strength, which usually depends on the size of particles with high variability. On the experimental side, only limited size-dependent strength data are available in the literature. Bieniawski [8] reported compressive strength of coal specimen for sizes ranging from 0.75 to 60 in. To the best of the authors' knowledge, strength data for much smaller particles (few hundred microns to mm scale) are not available in literature and are difficult to obtain due to a lack of appropriate test procedures for such length scales. It is also common to assume that particle strength follows some statistical law, e.g., Weibull distribution [53], with respect to particle size. Several researchers have assumed these distributions or other empirical laws to characterize the particle strength in their work [4,24–26,28,34,40]. The use of Weibull distribution for characterizing strength of brittle material as a function of particle size remains debatable [7].

In this study, the first approach based on the BPM is used to simulate coal particle breakage because of its algorithmic simplicity and the availability of experimental test data for calibrating bond strength. The particle breakage is modeled by constructing the macro-particles (or *agglomerates*) from the smaller sub-particles (or simply particles). The smaller particles are bonded together using a constitutive law, and the bond breakage between these particles constitutes the micro-fractures in the agglomerates. Several of these micro-fractures coalesce, eventually leading to breakage of the agglomerate into smaller fragments. The main objective of this work is to provide an integrated experimental and DEM-based computational framework to model the coal breakage and to examine effect of different operating conditions on the breakage rate. The application of this framework is demonstrated on a surrogate small-scale model with periodic boundary conditions. In this work, the particle-based open-source code Yade [50] has been used for the numerical simulations. The development of an *accurate* DEM to study the breakage of behavior of coal is not the focus of this work.

Note that the actual coal grinding process in mills also results in much finer particles or a powder-like substance, because of abrasion and chipping. The presence of such powdery material can have significant impact on the breakage behavior. The powder acts as a lubricant, leading to reduced intergranular force transmissions. Cleary [14] proposed a multiscale method to incorporate the effect of fine particles or interstitial powder in the DEM simulations. Any bulk motion or the powder lubricating effect is not accounted for in the current model.

The following section provides details on the constitutive laws and the DEM model used in this work. Section 3 discusses various parameters and material properties used to construct the model. It also covers the procedure for calibrating the bond strength between particles using the Brazilian Test. The model's capability in modeling breakage is then demonstrated on a small numerical sample of coal in Section 4. Because of the small model size and inherent assumptions in the boundary conditions, the model is currently not intended to provide quantitative validation for the coal particle breakage obtained through actual grindability operations. However, it provides a framework which can be expanded and utilized to study the effect of certain operating parameters on the mill efficiency. The main conclusions from this work are summarized in Section 5.

2. Model description

In this study, the soft-sphere approach of DEM [16] is adopted to capture the motion and interaction of particles. It consists of modeling an assembly of rigid, locally deformable particles that interact with each other by contact forces. Quite contrary to the common definition of "particles" in the field of mechanics as a point in the space, here it means a body occupying a finite volume of space. Only spherical particles are considered in this work, although other shapes are also possible. The classic DEM used in this work is based on an explicit numerical scheme. The contact forces and moments, governed by contact laws, are obtained at each time step using relative displacements and rotations of the particles. The updated positions of the particles are then obtained by integrating Newton's laws of motion.

In this study, the intact coal material is represented by a set of spherical agglomerates. Each agglomerate is composed of rigid spherical *particles* of radius 100 μm connected by cohesive *bonds*. Fig. 1 shows the example of an agglomerate consisting of several 100 μm spherical particles. The dense packing of spherical particles was obtained by isotropically compressing a much larger cubic sample of randomly arranged non-overlapping particles using rigid walls, to a resulting hydrostatic stress state of very small magnitude. This packing is then cropped to the desired spherical shape