



Parametrization and validation of a nonsmooth discrete element method for simulating flows of iron ore green pellets



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ABSTRACT

The nonsmooth discrete element method (NDEM) has the potential of high computational efficiency for rapid exploration of large design space of systems for processing and transportation of mineral ore. We present parametrization, verification and validation of a simulation model based on NDEM for iron ore green pellet flow in balling circuits. Simulations are compared with camera based measurements of individual pellet motion as well as bulk behavior of pellets on conveyors and in rotating balling drum. It is shown that the NDEM simulation model is applicable for the purpose of analysis, design and control of iron ore pelletizing systems. The sensitivity to model and simulation parameters is investigated. It is found that: the errors associated with large time-step integration do not cause statistically significant errors to the bulk behavior; rolling resistance is a necessary model component; and the outlet flow from the drum is sensitive to fine material adhering to the outlet creating a thick coating that narrows the outlet gaps.

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1. Introduction

Numerical simulation of granular materials is an important tool both for advancing the fundamental understanding of many natural phenomena in material science and geophysics, and for the design, control and optimization of systems for processing, manufacturing, storage and transportation of granular materials, e.g., grains, corn, pharmaceuticals pills, pellets, soil and minerals. In the mineral processing industry, experiments and in situ measurements are many times prohibitive for practical and economical reasons, and in these cases, modeling and simulation play an essential role in finding deeper understanding of the process, making radical improvements and innovating entirely new solutions.

Parametrization, verification and validation are critical steps for making sure that the simulation model provides a sufficiently accurate representation of the real system. By parametrization we mean the process of identifying numerical values of the model parameters from observations of the real system.

By the verification it is established that the computer simulation reproduces the mathematical model. A failure indicates either a flaw in

the numerical method or in the software implementation. Validation is testing the agreement between the simulated model and the real system. This determines the predictive power of the simulated model to some given degree of accuracy of a selected set of observables. A significant disagreement implies that the model is not useful for describing the systems behavior.

We consider the use of large-scale granular matter simulation based on the nonsmooth discrete element method (NDEM) [1,2] for the design of balling drum outlets [3] used in iron ore pelletizing [4]. The NDEM have the potential of high computational efficiency compared to conventional (smooth) DEM. This enables rapid exploration of the design space. The NDEM is on the other hand not as well tested as conventional DEM for industry applications and scarcely put to validation tests. In this paper we present procedure and results for parametrization of the properties of green iron ore pellets and validation of the macroscopic bulk behavior by comparing the numerical simulations with camera based measurements. The measurements include tracking of individual iron ore green pellets and characterization of bulk behavior in an industrial pelletizing system. The goal is to establish the predictive power of NDEM simulations for the purpose of design and control of pelletizing systems, including the sensitivity of the flow characteristics with respect to certain model parameters. The NDEM method in Ref.

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[2] is also extended to include a constraint based rolling resistance which is shown to be crucial for the material distribution of iron ore green pellets.

2. Background

2.1. Iron ore pelletizing

The iron ore pelletizing process usually has the following main stages [4]. Comminuted fine size ore, *finer*, is first mixed with binder material. Agglomeration into soft ore balls, *green ore pellets*, occur in balling circuits where fines, water and undersized pellets are fed into rotating drums. In the drum flow the green pellets are mixed with fine material and grow by layering and coalescence. New pellets are formed by nucleation. The drum is slightly inclined to produce an axial flow. The green pellets leave the drum through an outlet and are size distributed on a roller sieve, see Fig. 1. Under-sized particles are fed back to the drum. Over-sized pellets are crushed and mixed with the fines. On-sized pellets (9 to 16 mm in diameter) are conveyed to the induration furnace where they form hard pellets by oxidation and sintering. After this stage the cooled pellets are ready for transportation to distant steelmills. A typical iron ore balling circuit may have drum diameter ranging between 3–5 m and 8–10 m long and circulate about 400–1200 ton/h producing 100–300 ton/h on-size pellets.

The mathematical modeling of granulation systems was reviewed in Ref. [5]. A smooth DEM simulation model of iron ore granules in a continuous drum mixer was developed in Ref. [6] to analyze the flow dependence on drum design (angle and length). In Ref. [3] a methodology based on the nonsmooth discrete element method (NDEM) was presented for simulation based design of drum outlets, for even flow profile of ore green pellets on to the roller sieve. Fig. 1 shows an image from outlet analysis using NDEM simulation. The simulation demonstrates that the original outlet design was far from optimal as the material distribution on the wide-belt conveyor is inhomogeneous. As an effect, the roller sieve cannot be used efficiently. Furthermore, the green pellets may be damaged by the pressure from building a too thick pellet bed. A simulation model for the analysis and design of the balling process must be able to predict the flow and distribution of

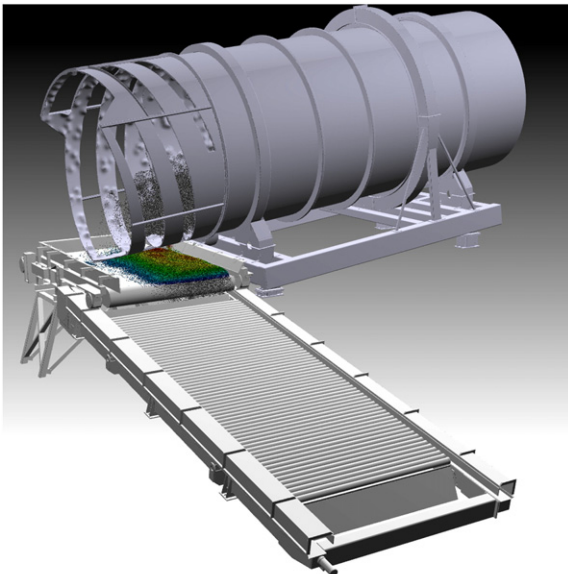


Fig. 1. Image from simulation of balling drum with green ore pellets flowing through the outlet gaps onto the wide-belt conveyor feeding the roller sieve.

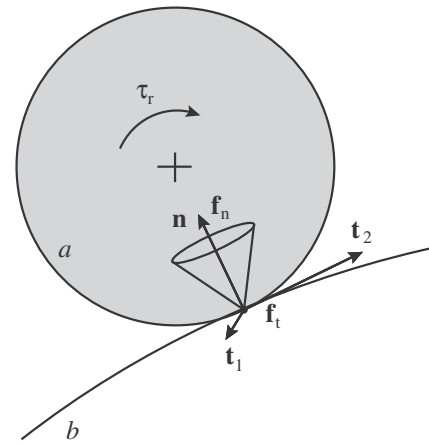


Fig. 2. Illustration of two contacting granular geometries *a* and *b*. Rolling resistance constraint produce a torque, τ_r , limited in magnitude relative to the normal contact force f_n in a similar way as the Coulomb friction force f_t .

material both inside the balling drum and on the conveyor belt below the outlet.

2.2. Nonsmooth discrete element methods

In the conventional discrete element method (DEM) the granules are modeled as rigid bodies interacting by contact forces modeled as linear or non-linear damped springs. We refer to this as *smooth* DEM as it involves the numerical integration of smooth (but usually stiff) ordinary differential equations. The computational aspects of smooth DEM are covered in Ref. [7]. In the *nonsmooth* DEM [8,9,1], impacts and frictional stick-slip transitions are considered as instantaneous events making the velocities discontinuous in time. The contact forces and impulses are modeled in terms of kinematic constraints and complementarity conditions between constraint forces and contact velocities, e.g., by the Signorini–Coulomb law for unilateral non-penetration and dry friction. The contact network becomes strongly coupled and any dynamic event may propagate through the system instantaneously. The benefit of nonsmooth DEM is that it allows integration with much larger simulation step-size than for smooth DEM and is thus potentially faster.

We use a regularized version of nonsmooth DEM referred to as *semi-smooth* DEM in Ref. [2], which combines the numerical stability at large step-size with the possibility of modeling the viscoelastic nature of the contact forces and mapping the simulation parameters to the conventional material parameters. The constrained equations of motion, between impacts, are

$$\mathbf{M}\dot{\mathbf{v}} + \dot{\mathbf{M}}\mathbf{v} = \mathbf{f}_{\text{ext}} + \mathbf{G}_n^T \lambda_n + \mathbf{G}_t^T \lambda_t \quad (1)$$

$$0 \leq \varepsilon_n \lambda_n + \mathbf{g}_n(\mathbf{x}) \perp \lambda_n \geq 0 \quad (2)$$

$$\gamma_t \lambda_t + \mathbf{G}_t(\mathbf{x})\mathbf{v} = 0 \quad (3)$$

$$|\lambda_t^{(\alpha)}| \leq \mu |\mathbf{G}_n^{(\alpha)T} \lambda_n^{(\alpha)}| \quad (4)$$

Table 1
Identified iron ore green pellet parameters.

ρ	3700 kg/m ³	Mass density
d	12.7 ± 3 mm	Diameter
E	6.2 ± 0.7 MPa	Young's modulus
e	0.18 ± 0.04	Coefficient of restitution
μ_s	0.91 ± 0.04	Surface friction coefficient
μ_r	0.32 ± 0.02	Rolling resistance coefficient

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