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A hierarchical simulation methodology for rotary kilns including granular flow and heat transfer

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ABSTRACT

Rotary kilns are used in several minerals processing operations, as well as related industries such as cement manufacture. Since they involve complex multiphase heat and mass transfer processes, optimization would ideally be guided by numerical modelling. A new generic hierarchical approach is proposed in this paper, sequentially combining 2D Discrete Element Method (DEM) simulations of slices of the bed and 3D two-phase computational fluid dynamics (CFD) models of the entire kiln, encompassing both bed and gaseous freeboard. DEM simulations have been used to derive mean solids velocities in a bed for various rotation speeds and particle sizes, and these were then used to calibrate and validate the solids rheology model used in the subsequent CFD model. A modified Coulombic friction for the bed in the CFD model was shown to give satisfactory agreement with the DEM bed results over a range of rotation speeds. Similarly, thermal mixing simulations carried out using the 2D DEM model for the granular bed were used to validate a CFD model of heat transfer after calibration of the small-scale diffusive term. The capability of the resultant CFD model was demonstrated by 3D simulation of the bed of a large rotary kiln.

1. Introduction

Many minerals processing operations utilize rotary kilns for processes such as roasting, calcining and nodulization. Examples include alumina calcining, the ilmenite reduction stage of the Becher process, iron ore reduction, and pet coke calcination.

Industrial applications of rotary kilns can be classified into four main types:

- Drying and pre-heating (including pellet induration)
- Calcination (eg. alumina, limestone, pet coke, TiO_3, etc)
- Mineral oxide reduction and other similar reactions
- Cement manufacture

Though there has been a trend in some applications towards the use of fluidized beds and suspension systems, kilns are still widely used.

Though rotary kilns are robust and the processes generally stable, issues such as ring accretion formation and minimization of energy consumption have been difficult to address decisively. Temperature distribution can be difficult to predict because reaction kinetics and heat transfer depend both on mixing of the solids in the bed, and on transfer between the bed and the gaseous freeboard space in which one or more flames will typically be located. In the Becher kiln, air injection into the kiln is staged along the length of the reactor so as to control temperature and oxidation degree. Such complexity of heat and mass transfer processes cannot be accounted for in simple models such as analytical expressions, empirical correlations, or even one-dimensional models. Detailed measurements are extremely difficult to make within a kiln, and even measurements of the solids and gas as they leave the kiln are very time consuming and expensive. Temperature measurements at the shell are similarly expensive, and all plant measurement attempts are problematic because of the inherent variability of kiln operations, and the long time-scales involved. Consequently, a numerical modelling approach is needed if optimization is to be carried out in a predictive way.

One dimensional models have been developed and applied for many years with some success in predicting global behaviour and quantities such as overall conversion (see, for example, Nicholson, 1995). However detailed information, such as would be required to avoid ring formation, requires a multi-dimensional modelling approach. Computational fluid dynamics (CFD) models are naturally suited to dealing with the gaseous freeboard including combustion processes, and can also be readily extended to incorporate heat transfer through the shell. Discrete Element Method (DEM) models are most naturally applied to

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modelling the granular bed, but the great length of many kilns, combined with the small particle size (ilmenite feed is typically less than 1 mm) and long timescales mean that practical design calculations using DEM to track every particle in an industry scale kiln is still computationally intractable for design purposes.

A new hybrid approach is described in this paper, hierarchically combining 2D DEM simulations and 3D two-phase CFD models of the entire kiln, encompassing coupled dynamics and thermal behaviour of both bed and gaseous freeboard. The approach has been demonstrated in this work: DEM simulations were used to derive mean solids velocities in a bed for various rotation speeds and particle sizes, which were then used to confirm the validity of the solids rheology model used in the CFD model, and calibrate the model parameters. This approach allows account to be taken of processes occurring at the particle scale as well as their contribution to processes occurring at the overall kiln scale over very long timescales. This is an example of a multi-scale approach, as described by Schwarz and Liu (2005), Liu and Schwarz (2009) and Schwarz et al. (2015). It should be emphasized that this hierarchical approach is quite different from the common coupled CFD-DEM technique in which the CFD component is used simulate the interstitial gas and DEM to simulate the granular solids. In the present hierarchical approach, the CFD and DEM modelling are carried out sequentially, rather than in the close-coupled concurrent way of the method commonly known as “CFD-DEM”. Furthermore, both CFD and DEM stages simulate the granular phase (at different scales), though the CFD component can also be used to simulate the interstitial gas when used in a two-fluid mode. The present approach is intended to be applicable to a wide range of different kiln processes, and takes advantage of the fact that CFD models are readily customized to incorporate specific flame types, specific gas-solids reactions, kiln internals, and so on.

2. Previous work on modelling rotary kilns

Only a limited amount of information appears in the literature describing detailed measurements of granular bed dynamics in plant or pilot plant operations, Nicholson’s (1995) work being an exception. On the other hand, there is a rich literature on solids motion in idealized cylinders, both horizontal and inclined (see, for example, Metcalfe et al., 1999). The axial motion closely follows plug flow, with significant mixing occurring in the transverse plane. Axial transport is well characterised both experimentally and theoretically, with formulas for residence time available, even for the situation with dam rings installed. While the motion in the transverse plane is well understood qualitatively, no simple methods to predict mixing and segregation exist.

Behaviour of a collection of particles in the transverse plane of a rotating cylinder can be categorized into one of six regimes: slipping, slumping/avalanching, rolling, cascading, cataracting or centrifuging. Of the six regimes only the first four are usually found in industrial rotary kilns. The mixing rate and potential for segregation is strongly influenced by the operating regime of the kiln bed. Parameters such as rotational speed, kiln diameter, percentage fill, friction between the wall and bed, and particle diameter and density determine the operating regime of the bed. DEM models have had considerable success in predicting these complex phenomena.

Mathematical models of kilns can conveniently be divided into two categories: one-dimensional process models which divide the kiln lengthwise into several slices or zones and carry out heat and mass balances on each zone; and multi-dimensional CFD and DEM models that attempt to solve for the gas and solids motion and chemical compositions at each point in the kiln.

2.1. One-dimensional models

In general, the 1D models can provide axial profiles of temperature, residence time, solids fill and gas composition along the kiln. Their advantage is short run times and that they can be tuned for a specific plant, thus allowing numerous changes in operating conditions to be quickly assessed. They can also be used in real time by operators by being incorporated into process control systems. A disadvantage of 1D models is that they are based heavily on plant operating data, making them only accurate over a limited range of operating parameters or for a specific application. Furthermore, they lack the ability to account for 3D details, and these are often important to kiln operation.

Thornton and Batterham (1982) describe a 1D phenomenological model of a rotary kiln used for processing iron-ore pellets. This model accounts for heat transfer by radiation and convection in the gas phase and solid conduction through the kiln wall. Motion of the solids is considered with heat transfer within the bed and from the bed to the gas and walls. This model was further developed by Thurlby (1988) and associated researchers. Boateng and Barr (1996) extended this concept of a 1D model by coupling it to a 2D transverse model that accounts for (transverse) bed mixing and segregation. Kritzinger and Kingsley (2015) showed how this type of 1D model can also be extended to account for multiple air jets (or flames) along the length of a rotary kiln, as is often used in pyrometallurgical minerals processing, e.g. in iron ore reduction. While such 1D models are clearly useful for design investigations, CFD simulations will undoubtedly be much more accurate for such complex multi-dimensional combustion processes where temperature and species concentrations are not uniform on transverse cross-sections, and more importantly, have transverse profiles that are dependent on their longitudinal position along the kiln. Similarly, DEM models will be able to better capture more complex granular bed phenomena such as size and density segregation. In some rotary kiln processes, gases are generated by reaction of solids in the bed, causing fluidisation of the particulate bed in some zones. Such phenomena cannot be captured in any way by a 1D model.

2.2. DEM models

DEM models typically focus on the dynamics of particle motion, simulating individual particle collisions, and are therefore valuable for elucidating the small-scale physics affecting bed dynamics. As a result, DEM simulations are expensive in computer time, particularly for industrial scale kilns with fine particles. Explicit integration of particle motion can also be a problem for systems with very long time-scales: thermal time-scales are extremely long for industrial rotary kilns. The Discrete Element Method is described by Cleary et al. (1998), Cleary and Sawley (2002) and Cleary (2004, 2009) in relation to various particle processing operations. It has particularly been used to explore size, density and shape segregation in slowly rotating 3D drums which have very similar bed dynamics to rotary kilns (Pereira et al. (2011, 2014) and Pereira and Cleary (2013, 2017)).

Finnie et al. (2005) studied longitudinal and transverse mixing in horizontal isothermal rotary kilns, using two and three-dimensional DEM. The focus was on the effect of the main operating conditions on quantitative measures of longitudinal and transverse mixing in short horizontal (i.e. non-inclined) rotating drums with a ratio of kiln radius to average particle radius of 40.0. While this is a valuable study for understanding trends, the particle size is very much larger than that used in industrial full-scale kilns, and the kiln is short: while it is long enough to capture some 3D effects, the aspect ratio is much smaller than that used in industrial kilns. The size of the simulation is thus very far from what would be needed for a realistic simulation of a full-scale industrial kiln. Kwapinska et al. (2006) analysed the details of transverse mixing between two populations of particles in a rotary drum using two-dimensional DEM simulations, comparing the results with experimental data, and pointing out that accurate prediction of interparticle mixing is needed for the models to be able to predict thermal behaviour in kilns. Chaudhuri et al. (2010) has demonstrated how such particle dynamics simulations can be extended to simulating heat transfer in rotary calciners.