Simulation of Roasting Metallurgical Concentrates in Fluidized Bed Using CFD-DEM

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Abstract. In this study, we utilized multiphase computational fluid dynamics (CFD), and discrete element method (DEM). Effect of the kinetic parameters of the roasting process in a fluidized bed was investigated. Our results indicate that it is possible to numerically integrate the coupled CFD-DEM system without significantly increasing computational overhead. It is also clear, however, that reactor operating conditions, reaction kinetics, and multiphase flow dynamics have major impacts on the roasting products exiting the reactor. We find that, with the same pre-exponential factors and mean activation energies, inclusion of distributed activation energies in the kinetics can shift the predicted average value of the exit gas-solid-phase and its statistical distribution, compared to single-valued activation-energy kinetics. These findings imply that accurate resolution of the reaction activation energy distributions will be important for optimizing roasting processes.

1. Introduction
Developing of coupling CFD-DEM models fluidized bed furnace requires careful consideration of the relevant physical processes: gas and particles dynamics of multiphase flow, the chemistry of the roasting process. The interaction between the phases must be properly taken into account for a realistic simulation. Laws that make up the mathematical formulation of each of these processes separately, are closely connected in a single system of equations[1].

Consideration of the various physical processes coupled together within one model, is quite a challenge for the simulation. On the other hand, this model will greatly improve the furnace roasting process by providing information on the desulfurization nickel concentrate, particle size distribution and compositions in the different zones of the furnace, in particular for the detection of high temperature zones, where there is excessive coarsening of the particles, resulting in the failure of the furnace.

Recently, computational models have provided considerable improvements due to high performance calculations using modern algorithms. A lot of CFD simulations using continuum models have been reported in literature [2,4,5]. However, these models show a serious over-prediction of the local heat transfer coefficient compared to experimental data and difficult formulation of constitutive equations (e.g. particle–particle drag) which may affect the simulation accuracy.

In this work, the multiphase phenomenon in liquid fluidized beds is studied by using the DEM-CFD method, which proved particularly promising [6,7] the fluid flow is obtained by solving the locally-averaged continuity and Navier-Stokes equations (CFD), while the motion of individual particles is studied by means of the Discrete Elements Method (DEM). This method presents the advantage of the capability to model liquids and particles properties and distribution [8].

There are mainly two typical multiphase CFD modeling techniques for studying fluidized bed processes, namely the Eulerian–Eulerian and Eulerian–Lagrangian approaches. In the Eulerian–Eulerian approach,
the two phases are treated mathematically as inter-penetrating continua and thus the approach is also called Two Fluid Model (TFM) [9]. Besides the fluid flow, an Eulerian framework is also applied to describe the motion of solid particles where the kinetic theory of granular flow (KTGF) is incorporated in most models to simulate particle collision for the closure of equation systems [9].

The advantage of the Eulerian–Eulerian approach is its superior computational convenience for multiphase flow. This gas–liquid–solid fluidized beds can be operated with different hydrodynamic regimes, which depend on the gas and liquid velocities, as well as the gas, liquid and solid properties. For proper reactor modelling, it is essential to know under which regime the reactor will be operating [10]. Two important hydrodynamic transitions within gas–liquid–solid fluidized beds are the minimum liquid fluidization velocity. The minimum liquid fluidization velocity is the superficial liquid velocity at which the bed becomes fluidized for a given superficial gas velocity; above the minimum liquid fluidization velocity, there is good contact between the gas, liquid and solid phases which is essential for heat and mass transfer processes [4,11,12].

2. Simulation models and methods

In the Eulerian–Eulerian approach, both gas and solid phases are treated mathematically as inter-penetrating continua. The basic idea is to use the governing equations correlating the changes of gas–particle flow in every computing unit to describe the properties of gas and solid phase. One does not have to monitor the trajectories of every solid particle. Therefore, Eulerian–Eulerian approach is one affordable modeling approach which could perform simulation of fluidized bed reactor at a pilot or industrial scale. For the sake of dividing the space occupied by solid and fluid, the concept of phase volume fraction (PVF) is introduced in this approach. The PVF is assumed to be continuous functions of space and time, and the sum of PVF of the gas and particle phase is equal to one [13]. This approach requires all processes at particle scale such as collision, drag, friction forces and heterogeneous chemical reactions to be solved in an Eulerian grid and included as phase interaction terms into governing equations.

Based on the Eulerian–Eulerian approach, the developed fluidized models could include hydrodynamics, heat transfer and chemical reactions together in multiphase systems. In order to calculate the transient nature of a gas–solid flow, the unsteady balance equations for mass, momentum, energy and species for gas and particle phases are solved. Meanwhile, different turbulent models are incorporated to compute the gas phase turbulent effect as well as reduce the computational burden. Granular stress equations based on KTGF are used to model the constitutive relations for the solid phase. When the solid phase is modeled as two or more continuous phase (different types or size), this model is called Eulerian multi-fluid/multiphase model. Obviously, the TFM is a basis of the multi-fluid model. The governing equations and reactive submodels below mentioned are generally used to develop the TFM for DPRS. The details of the model can be found in the cited literature [13,14].

3. Results and Discussion

3.1 Two-Way Coupling Simulation

In this work, method previously proposed [15–18] based on solving diffusion equations is applied to CFD-DEM simulations, where coarse graining is used to obtain solid volume fraction, particle phase velocity, and fluid-particle interaction forces. By examining the conservation requirements, the variables to solve diffusion equations for in CFD-DEM simulations are identified. The algorithm is then implemented into a CFD-DEM solver based on Ansys Fluent and ROCKY. The geometry of the computational domain considered in this study was a fluidized bed with a rectangular base, later it enables to calibrate the model with the laboratory stand of similar shape. At the first stage it was decided to simplify the task and does not take into account the heat transfer of solid material and other features conducted with the roasting process. The current Rocky formulation calculates the flotation and additional pressure gradient forces based on pressure derivatives extracted from the CFD solutions, which are exported from ANSYS Fluent.

In the momentum equation solved by ANSYS Fluent [7], the solution of the modified pressure field represents the static pressure variation due to the flow and the hydrostatic pressure at the reference
density, as given by Equation (2). The stress tensor is given by (3) were second term on the right hand side is the effect of volume dilation

\[
\frac{\delta}{\delta t} \left( \rho \mathbf{v} \right) + \nabla (\rho \mathbf{v} \mathbf{v}) = -\nabla p' + \nabla \bar{\ell} + \rho \mathbf{g} + \mathbf{\tilde{F}}
\]

\[p' = p - p_0 \cdot x\]  

\[\bar{\ell} = \mu \left[ \nabla \mathbf{v} - \nabla \mathbf{v}^T \right] - \frac{2}{3} \nabla\]

In a DEM CFD two way coupling simulation, the particles are part of the fluid flow and will affect it in a two-way interaction, i.e., the particle movement is affected by the interaction with other particles and the fluid around it while the flow is also affected by the particle presence.

On the Rocky side, the fluid flow will exert forces upon the particle, including pressure gradient (including buoyancy) force, drag force, and virtual mass force (optional). On the CFD side, the reaction of the forces upon the particles will be applied over the fluid phases. The scheme used in the Rocky DEM CFD two-way coupling module allows both solvers to run in parallel, which can considerably decrease simulation time if the solvers do not compete for resources. During setup within the Rocky coupling module interface, you can control the number of processors required by each solver to avoid resource competition.

![Figure 1](image-url)

**Figure. 1** Mixing behavior of particles in fluidized bed with 3 injectors simulated

The Rocky DEM-CFD two-way coupling module uses a neighbor cell averaging procedure to avoid high volume fractions in a certain cell of the CFD domain, distributing the volume of the particles that are positioned at the cell boundaries among the adjacent cells. Thus, this methodology is suitable for dealing with a large number of particles within a CFD cell and not for dealing with particles larger than the CFD cell. Therefore, it is recommended that the mesh size be larger than the largest particle size.
throughout the simulation domain. Some regions with detailed geometry and strong gradients can have smaller cells but the coupling results in these regions will be less accurate. As you can see from Fig. 1 shows the result of a computer simulation conducted using the CFD-DEM approach to investigate mixing behaviors during fluidization of solid particles (~400,000 spherical particles). The particles were differentiated by their colors in the absolute translational velocity. Particles were re-distributed rapidly and good mixing was achieved after a short period of fluidization. Such behaviors may be attributed to the presence of relative dynamic motions between particles that were induced by the flow of gas through the granular bed.

4. Conclusions
Analysis of the results shows how the various processes are closely related in the furnace. Results of the model show intensive circulation of solid and gas phase inside the furnace. Influence of solid phase at blast volume is a fairly obvious fact, as this is one of the key factors in relation to the placement of the blow injectors.

Computational studies of mixing behaviors of granular materials in gas fluidized bed systems also were conducted in this study. Methods of improving fluidized bed modeling in such systems, such as through different methods of air injection, varying the geometry of the fluidized bed, including the calculation of heat exchange between the gas and solid material, particle size distribution of various fractions, destruction and agglomeration of solids, are possible subjects of future studies.

Determination of the optimal design of the furnace, the charging device, blow nozzles, including a better understanding of the processes occurring in the furnace will allow directly to minimize the risk of excessive sintering of particles, reduce the residence time of the particles inside the machine, improve product quality, and reduce the amount of waste gases.

High temperature industrial processes is a challenge for numerical simulation as you have to take into account the multi-phase flows, interacting with each other. Recent developments within the CFD-DEM simulations allow us to consider these processes on an industrial scale in one model.

These results demonstrate how CFD model does not correspond to the actual roasting process, however this model is an important development tool for the further investigations of this type of production process. The results will provide representation for operation of existing facilities and create conditions for the design of more efficient industrial furnaces with low emissions and improved technical and economic performance.

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