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SIMULATION OF REACTING MOVING GRANULAR MATERIAL IN FURNACES AND BOILERS

AN OVERVIEW ON THE CAPABILITIES OF THE DISCRETE ELEMENT METHOD

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Abstract

A brief overview is given on the capabilities and on the current limitations of the Discrete Element Method (DEM) coupled with Computational Fluid Mechanics (CFD) to simulate chemical reacting moving granular material. An approach to resolve the internal transport and reaction phenomena in particles of complex geometry is presented. Heat and mass transfer from and to the particles are accounted for as well as heat transfer between particles and between particles and a surrounding gas phase including radiation. Gas phase reactions outside the particle interact with inner particle processes.
Examples will be shown to demonstrate the capabilities of DEM/CFD coupling. These examples are an industrial scale lime shaft kilns, the simulation of a domestic pellet stove and a grate firing system for the incineration of municipal waste. The advantages of a DEM/CFD approach will be highlighted but also the still existing drawbacks and limitations are discussed. The paper ends with an outlook on necessary developments to make DEM/CFD a standard engineering tool for chemically reacting granular material.

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Keywords: granular material; reaction; combustion; DEM; CFD

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1. Introduction

The thermal processing of relatively large particles is a common task in industry. Typical examples are the calcination of limestone, dolomite or magnesite in shaft kilns, the production of foamed clay in rotary kilns, the conversion of iron-oxide particles in blast furnaces and the combustion of pellets, wood chips or municipal waste on grate systems. All these systems of industrial scale face common difficulties which makes the numerical description of such systems extremely challenging:

- particles are rather large in the cm range indicating that internal gradients of temperature and composition cannot be neglected in modelling,
- particles are typically of complex shape (e.g. wood pellets or chips) and underlie a particle size distribution which influences the particle movement in the systems and can lead to phenomena like segregation, arching and bridging,
- particles can change their shape and size during thermochemical processes like combustion over time,
- the number of particles can easily reach millions.

In many applications the particles are in contact with a surrounding gas phase passing through the granular assembly. These gases can be air (cooling or combustion air), gases released by the particles (volatiles from solid fuels, CO_2 from calcination) or a gaseous fuel which delivers heat for endothermic particle processes (e.g. calcination).

The question arises what kind of simulation approach is able to describe the relevant multi-physics phenomena in such systems reflecting the granular nature of the material to be processed. The most common approach is to approximate the granular material as a continuum which allows acceptable computational times and is very often justified for large industrial systems. A next step is to use continuum approaches in combination with models based on representative particles. Population balances are often used when very large particle numbers are of interest. However, all these approaches cannot reflect effects on the bulk movement like arching, segregation, inner particle processes, influence of complex shapes and wide particle size distributions in a reliable way.

A method which, in principle, is able to describe the phenomena mentioned is the Discrete Element Method (DEM). DEM tracks the movement of each individual particle in a granular system and its interaction with other surrounding particles or walls. DEM is an emerging scientific method with fast growth. Throughout the last five decades DEM evolved from the even older concepts of Molecular Dynamics (MD). For its application in the context of solid spherical particles the work of Cundall and Strack [1] may be considered as the starting point while the consideration of actual particle geometries is (at least for large numbers of particles) a recent development [2]. For many problems without chemical reaction like bulk handling or geological questions it became a standard engineering tool. Commercial tools like EDEM or Ithasca or open source codes like LIGGGHTS are available. There, coupling with CFD is also possible to describe, for example, processes in fluidized beds [3][4][5][6].

However, as soon as chemical reactions in such systems have to be accounted for the number of publications is still rather limited [7][8][9][10][11][12] and the situation gets even worse when the particles are large and/or of complex shape.

Peters [13] was among the first to consider chemically reacting large particles within the DEM context, already in the late 90ies. He currently works mainly on the pyrolysis and combustion of biomass in fixed beds and on grate firing systems [14][15][16]. Wu et al. [17] did simulate gas-solid reacting flows in fluid catalytic cracking processes. Sun et al. [18] examined raceway phenomena with DEM/CFD. Radl et al. [19] presented PARSCALE, an extension to LIGGGHTS, to account for intra-particle heat and mass transfer and presented as an example the oxidation of porous copper particles. Kuwagi et al. [20] presented an approach to describe the incineration of Caesium containing nuclear waste in a fixed bed reactor by CFD/DEM. Our one group did use DEM/CFD to simulate drying of wood chips in a rotary kiln [21], the combustion of wood pellets in a domestic heating system [22], the calcination of limestone in shaft kilns [23][24] or the combustion of municipal waste on grate firing systems [25]. Note that most of these publications, except Sudbrock et al. [26] and Wiese et al. [22], are limited to spherical particles.