Extended Discrete Element Method (XDEM) to Model Heterogeneous Reactions in Packed Beds

F. Hoffmann[1], B. Peters[1]
[1]University of Luxembourg, Luxembourg, Luxemburg

Packed beds, due to their high surface-area-to-volume-ratio, are widely used for chemical reactors, such as catalytic or pebble bed reactors, blast furnaces or as heat exchanging units. Depending on the mode of packing, structured or random, a different degree of heterogeneity is introduced. For stable and efficient process handling local quantities such as temperature or concentration of chemical species are of major interest. Direct measurement of such quantities has proven very difficult or unfeasable due to the morphology of the bed. Hence, numerical modeling can help to gain insights into inaccessible parts of such reactors.
The objective of this contribution is to introduce a discrete numerical approach that describes heterogeneous reaction processes within packed and moving beds. The so-called Extended Discrete Element Method (XDEM) is used to account for convective heat and mass transfer within porous media. Both motion and chemical conversion of particulate material can be dealt with. A granular medium consists of an ensemble of particles of which each exhibits individual chemical and mechanical properties. Dynamics of solid particles is accounted for by the known discrete element approach. In addition physicochemical conversion of an individual particle like drying, gasification or redox reactions are accounted for by transient differential equations (species, energy, momentum) on a particle scale. Predictions include properties such as temperature and species distribution inside a particle. The general and modular formulation of the model allows for application to any chemical process involving heterogeneous reactions. Chemical interaction between multiple particles takes place through gaseous intermediates by heat and mass transfer. Computational Fluid Dynamics is applied for the gaseous continuum in the voidage between particles.
The presented model can act as tool to gain valuable insights into chemical processes inside packed beds such as blast furnace iron making or gasification of biomass. It can serve as a toolbox for prediction, analysis and optimization of a variety of process parameters such as residence time, conversion progress, burden charging and gas flow patterns. As an example a section of the burden in a blast furnace is focused on.