

K1-MET

Competence Center for Excellent Technologies in Advanced Metallurgical and Environmental Process Development

Programme: COMET – Competence Centers for Excellent Technologies

Programme line: K1-Centres

COMET subproject, duration and type of project:

Bulk solids modelling, 07/2015 –06/2019, multi-firm

Direct reduction of Iron Ore

Iron ore is usually reduced to directly reduction iron (DRI) by using coal (C,CO) or hydrogen. During the previous K1-Met period a detailed single particle model for this reduction process has been developed and validated against single particle measurements. In this project, we developed a comprehensive model for the simulation of direct reduction of iron ore within fluidized beds. Here, the hydrodynamics of the poly-dispersed fluidized bed is captured by a hybrid model, which has recently been successfully applied to industrial cyclone separation as well as bi-disperse fluidized beds, while the reduction model can be applied on a particle base. Our simulations reveal qualitatively well the reduction of iron ore in fluidized bed reactors.



Introduction

Fluidized bed and moving bed reactors are one of the most important technologies in several branches of process industry (polymer production, carbon capture, direct reduction of iron ore, fluid catalytic cracking (FCC), biomass reactors). Especially, it is known since decades that iron can be reduced rapidly and efficiently from iron carrier materials using such devices. The primary energy sources and reducing agents are CO and H₂, which are finally released as CO₂ and H₂O to the environment, respectively. Since iron reduction consumes about 70% of the energy during steelmaking, it can be considered as core process in steel industry. Due to the limited accessibility for measurements, simulation methods have become one of the most important tools for optimizing the iron making processes, such as the blast furnace, the FINEX fluidized beds as well as the shaft furnace moving beds.

Here, one faces two major challenges. On the one hand, the hydrodynamics (i.e. mixing, gas-solid contact) has to be captured appropriately

as well as efficiently, since these processes typically contain billions of particles. On the other hand, the complex chemical processes determining the reduction of single iron ore particles have to be accounted in such a simulation of the industrial process.



Numerical simulation of polydisperse fluidized beds

In this project, we therefore developed a hybrid simulation methodology, which employs a combination of a Lagrangian discrete phase model (DPM) and a coarse-grained two-fluid model (TFM) to take advantage of the benefits of those two different formulations. While the DPM model unveils the local particle size distribution, TFM accounts for the particles stresses. Furthermore, sub-grid modifications account for the small heterogeneous structures, which are not resolved in the case of coarse grids required for industrial scale simulations.

Figure 1 shows the segregation in a bi-disperse fluidized bed. The numerical results are in fairly good agreement with experimental data, but

require considerably less computational resources compared to state-of-the-art modelling approaches.

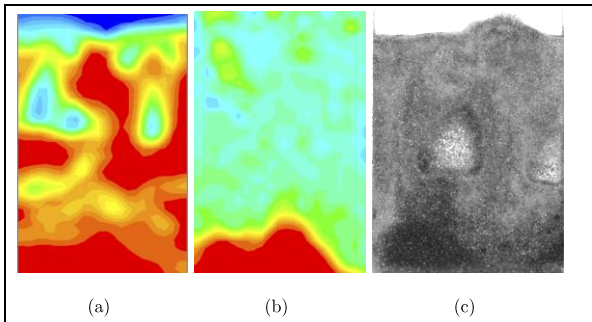


Fig. 1: Snapshots of a) solids volume fraction (blue: no particles; red: maximum packing), b) the fraction of large particles and c) photograph of experiment.

Direct reductions of Iron ore

This hybrid approach further enables the efficient evaluation of gas-solid reactions at a particle level using DPM.

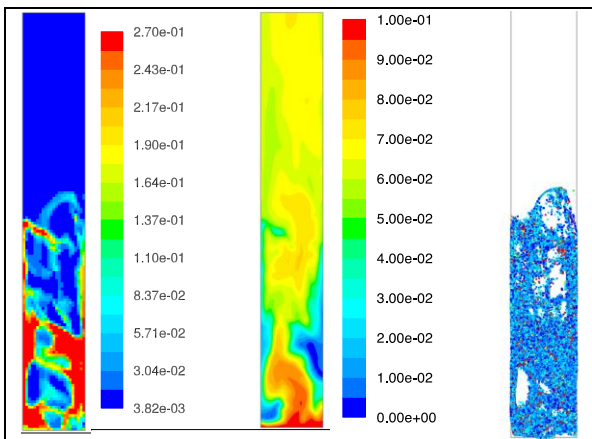


Fig. 2 left: particles volume fraction; middle: mass fraction of CO; right: iron ore tracer particles color by degree of reduction.

Here, we employed a single particle model for the direct reduction of iron ore developed at the Institute for Energy Systems and Thermodynamics (TU Vienna) within the previous K1-MET period. For example, figure 2 shows the consumption of CO in a fluidized bed due to the reduction of magnetite to hematite, which results into an increase of the degree of reduction with time (figures 2 and 3).

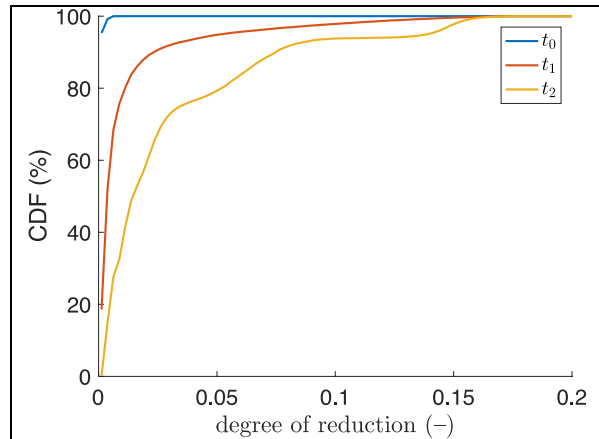


Fig. 3: Degree of reduction as a function of time.

Impact and effects

In this project we successfully combined the scientific work of different K1-Met partners and developed a hybrid model, which combines the efficient evaluation of the hydrodynamics of a fluidized bed with the detailed analysis of particle based reactions. This enables highly efficient simulations of this multi-scale process. It is noteworthy that this methodology by its own is generally applicable to different disciplines beyond metallurgy as, for example, to polymer industry.

A deeper metallurgical understanding of the direct reduction of iron ore in fluidized beds, in turn, enables the design of such processes.

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