Modelling of Chemical Reactions in Metallurgical Processes

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ABSTRACT

Developing ways for the direct reduction of iron ores has attracted much research interest in the last three decades, since it can be considered as a core process in steel industry [1]. One of the most advantageous direct reduction processes are fluidized bed reactors. However, due to the harsh conditions inside these reactors, most investigations are carried out through computational tools. One of these tools is the CFD-DEM method, in which the gas phase reactions and governing equations are calculated in the Eulerian (CFD) side, whereas the particle reactions and equations of motion are calculated in the Lagrangian (DEM) side.

In this work, the CFD-DEM method is extended to cover the most common types of representation models for the reactions of solids submerged in fluids. These models are the Shrinking Particle Model (SPM) and the Unreacted Shrinking Core Model (USCM) [2].

With the use of the SPM, the implemented communication framework between the CFD and DEM sides have been verified by running some preliminary cases and comparing the species mass balances. Since, in the metallurgical process of iron-ore reduction, in which the oxygen is extracted from the iron-oxide through intermediary steps, the SPM would be insufficient. In this case, one must consider the different reaction steps, therefore a three-layered USCM representation proves to be a realistic fit [2, 3]. The different layers can be described from outermost to innermost as Fe, FeO, Fe_3O_4 and Fe_2O_3, which is the innermost core of the particle. The gaseous reactant diffuses through the porous layers of iron shell (Fe), wustite (FeO) and magnetite (Fe_3O_4) layers, while simultaneously a portion of the diffused gas reacts at layer interfaces, and the rest of the reactant gas continues its diffusion through the other layers until the hematite (Fe_2O_3) core of the particle is reached. Once the core is reached, the gas reacts with the hematite at the surface and produces magnetite. For the investigation of metallurgical processes both of the mentioned models is implemented into the CFD-DEM library in such a manner that only the required data is communicated between the two phases with an adaptable communication interval. The implemented USCM for the iron-ore reduction is validated by constructing a simple computational domain consisting of a single iron-ore particle. The model is then validated by comparing the overall reduction rate of the particle with available literature.

REFERENCES

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