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Determination of Kinetic Parameters for Heterogeneous Reaction System Employing Discrete Element Methods under HPC Platforms

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The complex processes of heterogeneous reactions of granular materials such as occurring during metals-ore reduction or biomass gasification involve numerous physical phenomena. The combination of elevated temperature, complex flow, aggressive atmosphere and heterogeneous chemistry make it difficult to study these industrial processes. One of the most important aspects of heterogeneous reactions is to understand and quantify the evolution of the different transformations. For instance, during metal-oxides reduction processes, it is of high importance to quantify the rate at which the pure metal is formed. Nevertheless, it is almost impossible, by experimental means only, to separately observe, accurately quantify and gain insight into these mingled nonlinear physical and chemical processes. In the last decade, numerical simulation tools for particulate processes, such as the eXtended Discrete Element Method (XDEM), have become indispensable to study complex systems without the need of costly experimental practices. In the past, the XDEM has been employed to predict the reduction of tungsten trioxide (WO_3) in dry hydrogen (H_2) atmospheres [1] and reduction of iron ores [2]. In the before-mentioned research works, it was employed kinetic data extracted from literature. On one hand, in these processes the kinetic data differ from each other. This is due to the fact that the experimental data in the literature is interpreted with lumped models and empirical models bonded to the specific experimental conditions. On the other hand, advanced simulation tools, such as XDEM, account for all the influencing phenomena (e.g. species and energy distribution, flow conditions, particles shape, rheological properties) constantly interacting in time and space. In these advanced simulation tools, each particle is treated and solved as individual entities and an accurate prediction of the species formation and transport in time and space is provided. Thus, in such advanced numerical tools, the reaction rate parameters representative of the kinetics alone of the involved chemical reactions must be employed.

In this contribution, two XDEM simulation case studies accounting for the industrial reduction of WO_3 are presented. The first case study is employed to determine the reaction rate parameters of the four prevalent reduction steps ($WO_3 \leftrightarrow WO_{2.9} \leftrightarrow WO_{2.72} \leftrightarrow WO_2 \leftrightarrow W$) upon the H_2 reduction of WO_3. Where the reaction rates are modeled following an Arrhenius law with two parameters per step (i.e. pre-exponential factor and activation energy). The constituted optimization problem of minimization of error of the XDEM simulations vs experimental data, implemented and solved in a High Performance Computing (HPC) cluster, is presented and discussed. The determined parameters are later assessed by comparison to a secondly presented case study.

References

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