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Editorial: Understanding the behavior of reactive solid materials in chemical processes

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Editorial on the Research Topic
Understanding the Behavior of Reactive Solid Materials in Chemical Processes

Reactions on solids is a rather complex, but very important area in the field of Chemical Reaction Engineering, as they are in the core of large-scale industrial sectors such as hydrometallurgy, and biomass valorization. The reactive solids behavior influences greatly the overall reaction kinetics and thus, process efficiency and economics and understanding the factors influencing this is the key for process development and fundamental understanding. Typically, the diffusion of material influences significantly the overall reactivity and the system is also dynamic, as the interacting solid particles may change in geometrical shape during the reaction–therefore the interpretation of kinetics need to be tackled by understanding advanced phenomena and models that describe the change in parameters including shape and surface area. In this special issue, many of the often-encountered scenarios dealing with solid-fluid reactions have been discussed from different angles and methods for overcoming the complexity of a solid-liquid or solid-gas system have been presented.

In the perspective article by Salmi et al., the short historical endeavor of solid reaction theory is discussed, and the theory dealing with non-ideal surfaces in a solid-fluid system is thoroughly explained along with the governing mathematical expressions. The approach presented here can be used to describe kinetics of non-ideal solids having surface defects and ultimately the model approaches the model used for completely porous particles. The importance oif the shape factor is thoroughly discussed and emphasized that the main benefit of including non-ideality is to get better kinetic models.

In the article by Julcour et al., it was demonstrated how Nickel Slag Carbonation in a Stirred Bead Mill, which is an attrition-leaching carbonation process, can be studied and different modeling approaches are explained in detail. They developed an original thermo-kinetic modelling approach, which combines equilibrium thermodynamic

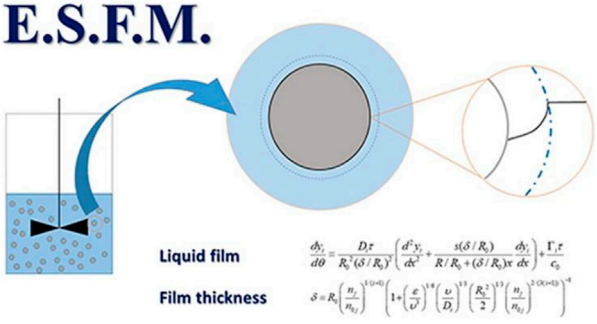

FIGURE 1
The extended shrinking film model illustrated by Russo et al.

models with particle reaction kinetic models, to get a better understanding on the mechanisms in this process.

Russo et al. analyzed the possibility to adopt rigorous fluid-solid models for the special case of shrinking reactive particles by applying of the so-called extended shrinking film model (ESFM) (see Figure 1). The model considers several physical phenomena: the reactive solid dissolution in the liquid phase, the radial shrinking of solid particles vs the reaction time, and radial dependency of the liquid film surrounding the particle, through which the liquid component diffuses to react with the dissolved solid. Additionally, non-ideal shaped particles were also considered when developing the model by including the shape factor. The model was tested in several conditions and the results appear to be rather general and flexible to be applied to a wide range of chemical systems.

Niidu et al. presented a complex practical case study dealing with oxidative leaching of organics from an inorganic matrix in the article "Behavior of Estonian Oil Shale in Acidic Oxidative Conditions". The aim is to simultaneously extract and steer the selectivity of the products during the reactive extraction. The results clearly indicates that high yields, around 90% of carbon present in the initial oil shale, can be obtained when utilizing process optimization, which enables the employment of this valuable raw material for higher value added chemical production compared to energy production, which is its main current use. The work is related to the highly topical theme of utilizing oil shale for purposes other than energy production, which is of high economic importance in several parts of the world including Estonia.

Finally, Hilpmann et al. investigated the reaction Kinetics of one-pot xylan conversion to xylitol via metal catalyst, namely Ru/C, underlying that the one-pot process can be an efficient alternative to the classical two-step process where hydrolysis is put in series with hydrogenation. The kinetics of the reaction was thoroughly investigated–three different mathematical models were described and their prediction accuracy discussed. The first one, a generalized second-order model displayed a mean error of over 4% and curves were only satisfying at a narrow range of temperature. The second attempt was a complex model in order to improve the fit for both xylitol and xylose and it combined hydrolysis kinetics (via acid-base catalysis) with Langmuir–Hinshelwood kinetics for the Ruthenium powder catalyst. However, the mean error increased slightly compared to first model with this approach. The final, third model, was a vigorous refinement of the complex model and most reliable at a larger temperature range.

Author contributions

All authors listed have made a substantial, direct, and intellectual contribution to the work and approved it for publication.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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