Chemical Reaction Engineering: Looking towards the Future from a Molecular Perspective

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Abstract

During the latter half of the twentieth century, the field of chemical reaction engineering made continuous advances in the development of methods for describing the performance of chemical reactors. The development of progressively more efficient and robust methods for solving large sets of partial differential equations and for handling complex reactor geometries and boundary conditions have been essential to achieving these advances. The solution of larger and more complex problems has been enabled, as well, by in advances in computer speed and memory. The past twenty years have also witnessed the development of increasingly accurate and efficient methods for the prediction of adsorption isotherms and diffusion coefficients for molecules in a various micro- and mesoporous materials and for the prediction of the reaction energetics and dynamics from first principles. As a result, it has become possible to think about chemical reaction engineering from both a molecular and a macroscopic perspective. Construction of the bridges between these perspectives has begun to occur, and one can now envision a future in which it will be possible to explore the performance of reactors, beginning with a molecular understanding of the reactants and catalysts together with inputs about the pore structure, connectivity, etc. of the catalyst and the geometry and flow configuration of the reactor. This talk will illustrate some of the advances made in the in the ab initio prediction of reaction kinetics and molecular transport, and will show how such knowledge can be combined to predict catalyst performance at the catalyst pellet level.