
Virtual Process Engineering via Multi-Scale Discrete Simulation — from reactions to reactors

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Abstract

Discrete elements present ubiquitously at multiple scales in chemical engineering, from atoms and molecules to particles, droplets and bubbles. Discrete simulation based directly on the description of these elements is, however, not used as common in engineering. In this talk I will demonstrate that by reasonable coarse-graining and coupling of models at different scales, discrete simulation could become an accurate and efficient tool for virtual experiments and tests on practical systems. Taking full advantage of state-of-the-art supercomputing, it may even bridge the vast gap between reactions and reactors, fulfilling the ultimate goal of chemical engineering.
