

**Multiscale simulation on adsorption processes:
state-of-arts**

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This study presents a multi-scale simulation method starting at the molecular level for adsorption processes. The multi-scale simulation includes i) molecular-level simulation (MLS) in micro-pores, ii) micro-fluid-level simulation (mFLS) for flow dynamics in macro-pores, iii) fluid-level simulation (FLS) within adsorption column using CFD (computational fluid dynamics), and iv) process-level simulation (PLS) for optimization of operating conditions and design parameters.

In this talk, we overview the state-of-arts of multiscale simulation (MSS) and present how to apply MSS to adsorption process development. Simulated moving-bed (SMB) is taken as an example for the application.