Multi-scale simulation starting at the molecular level for p-xylene adsorption process development

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This research aims to develop a multi-scale simulation method starting at the molecular level for p-xylene simulated moving bed (SMB) separation process. The multi-scale simulation includes i) molecular simulation of xylene isomers adsorption on zeolite and diffusion in pores, ii) micro-fluid dynamics in pores, iii) fluid dynamics simulation within adsorption column, and iv) SMB process simulation for optimization of operating conditions and design parameters.