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Interplay between restricted transport and catalytic reaction in nanoporous materials: KMC simulation and analytic theory ANDRES GARCIA, JING WANG, DAVID ACKERMAN, JAMES EVANS, Iowa State Univ — Behavior of catalytic reactions in narrow pores is controlled by a delicate interplay between fluctuations in adsorption-desorption at pore openings, highly restricted diffusion, and reaction. The resulting concentration profiles determined by KMC simulation, showing reactants mainly near pore openings, are not described by standard mean-field reaction-diffusion equations. For simple A→B unimolecular reaction kinetics, the challenge in developing a correct theory is to suitably describe chemical diffusion in mixed-component quasi-single-file systems. This is achieved based on a refined picture of tracer diffusion for finite-length pores. For A+B→C+D bimolecular and other reactions, there are additional complications in describing spatial correlations in reactant locations which can strongly impact the reaction kinetics.

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