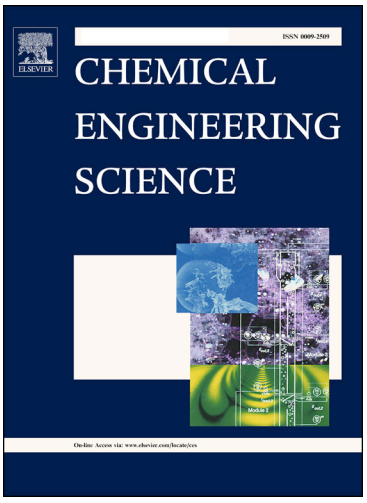

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Efficient Simulation and Equilibrium Theory for Adsorption Processes with Implicit Adsorption Isotherms - Ideal Adsorbed Solution Theory

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Abstract

Recently an efficient method for the simulation of packed bed adsorbers with implicit adsorption isotherms was presented. It uses a method of lines approach and exploits standard software for the simultaneous solution of the resulting differential algebraic equations (DAEs). Application was demonstrated for stoichiometric ion exchange. In the present paper, the approach is extended to systems described by the adsorbed solution theory. For that purpose, the relation between the differential index of the DAE system and the spectral properties of the underlying adsorption equilibrium is established. In particular, it is shown that real and positive eigenvalues of the Jacobian of the underlying conservation equations will lead to a differential index of one. It is further shown that real and positive eigenvalues of the Jacobian related to the IAST can be guaranteed for binary mixtures with any type of pure component adsorption isotherm or for multicomponent mixtures with certain restricted types of pure component isotherms. The new method is illustrated for different explicit and implicit pure component adsorption isotherms belonging to this class. It is compared with alternative solution approaches using the modified FastIAS method by Do and Myers and semi-analytical solutions from equilibrium theory.

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