Modelling ion exchange kinetics in zeolyte-type materials using Maxwell-Stefan approach

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ABSTRACT

In this essay, the Maxwell-Stefan (MS) formalism was adopted to model the removal of cadmium(II) and mercury(II) ions from aqueous solutions using microporous titanosilicate ETS-4. The embodied transport mechanism is surface diffusion, since the small pore diameters of such zeolite-type materials imply that counter ions never escape from the force field of the matrix co-ions, mainly owing to the strong and long range electrostatic interactions. The parameters of the global model are the MS diffusivities of ion–ion and ion–solid pairs, and a convective mass transfer coefficient. The average absolute relative deviations (AARD) achieved for Cd²⁺/Na⁺/ETS-4 and Hg²⁺/Na⁺/ETS-4 systems were only 3.47 and 7.34%, respectively. The model calculates concentration profiles and their evolution along time under transient regime, being able to represent the initial steep branches of removal curves and subsequent transition to equilibrium, where kinetic curves are frequently very difficult to fit. The well-known and frequently used pseudo-first and pseudo-second-order equations were also chosen for comparison, and provided large deviations: AARD(Cd²⁺) = 48.9% and AARD(Hg²⁺) = 26.6 % (first order), and AARD(Cd²⁺) = 29.0% and AARD(Hg²⁺) = 54.6% (second order).

Keywords: Ion exchange; Kinetics; Modelling; Maxwell-Stefan; Diffusion; Titanosilicate