Jordan University of Science and Technology

Modeling solute transport affected by heterogeneous sorption kinetics using single-rate nonequilibrium approaches

Authors: Munjed A. Maraqa and Saud A. Khashan

Abstract: Single-rate transport models are commonly used for interpreting sorption-related mass transfer in porous media, often with the intention of approximating the kinetics of the sorption process. Among the most commonly used single-rate models are the two-site first-order (TSFO) and the two-site radial diffusion (TSRD) models. We fitted the parameters of the TSFO and TSRD models to simulated breakthrough data of hypothetical column experiments in which sorption rates were described by a ?-distributed sorption sites (GS) model. Our objective was to determine the conditions under which the assumption of a single-rate sorption parameter will be applicable to systems with heterogeneous sorption rates. We were further interested in knowing in what manner the fitted single-rate nonequilibrium model parameters depend upon the conditions under which the data were obtained. The considered hypothetical cases covered a range of experimental conditions and involved compounds with different sorption characteristics. The study revealed that the goodness of fit of the single rate models in simulating the transport of solutes exhibiting heterogeneous sorption rates is affected by solute residence time and pulse injection duration. Compared to the TSFO model, the TSRD model generally results in better prediction of solute transport affected by heterogeneous sorption kinetics. In addition, for such systems, the nonequilibrium parameters fitted using the TSFO model and their counterparts in the TSRD model are highly correlated. Moreover, an increase in the fitted mass transfer timescale of each of the single-rate models is coupled with an increase in the associated fraction of instantaneous sorption sites. A strong correlation was found between the time of the experiment and the product of the fitted characteristic time for mass transfer, pulse duration, and solute residence time. The correlation explains many of the variations in the mass transfer timescale encountered when single-rate s