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HIGH ACCURACY NUMERICAL SOLUTION OF AN ADVECTION–ADSORPTION MODEL WITH FREUNDLICH OR LANGMUIR ISOTHERMS

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ABSTRACT

For the numerical solution of a system of nonlinear advection-adsorption partial differential equations, we develop a semi-implicit finite difference scheme with a second-order spatial discretization error. The mathematical problem arises from the domain of water purification using activated carbon. We are particularly focused on a use-case involving the simulation of fixed-bed adsorption process for the removal of organic micropollutants from drinking water. The implicit approximation of part of the system's equations is needed due to some specifics of the values of model parameters. Our aim is to accurately simulate the outflow concentrations of the adsorbates. This, in turn, allows for the precise computation of breakthrough curves, which are key indicators in evaluating the effectiveness of water treatment.

The mathematical model is capable of describing both single-component and multi-component adsorption processes. In the single-component adsorption scenario, we examine two formulations of the model—one utilizing the Freundlich isotherm and the other based on the Langmuir isotherm to represent the adsorption term. Incorporating various isotherm equations into the mathematical model enhances its flexibility and enables the simulation of a broader range of adsorbate–adsorbent systems. In the multi-component case, the numerical method is effectively applied to simulate breakthrough curves for up to ten contaminants.

The proposed finite difference scheme is analyzed through numerical experiments, demonstrating its effectiveness across various parameter settings and confirming second-order convergence with respect to spatial discretization. A comparison is made with a first-order numerical scheme applied to the same problem, highlighting the advantages of the newly proposed method. In particular, using the latter, it is shown that the maximum approximation error for the concentration of contaminant, relative to the inlet concentration, does not exceed 10^{-6} in magnitude.

Keywords advection-adsorption · numerical simulation · breakthorugh curve · Freundlich isotherm · Langmuir isotherm

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