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Incorporating Core-Shell Particles using a Two-Dimensional Non-Equilibrium Chromatography Model

Communication Info

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Abstract

The study numerically solves a nonlinear, non-isothermal, two-dimensional lumped kinetic model (2D LKM) to simulate the transport behavior of multi-component mixtures in fixed-bed liquid chromatography columns packed with core-shell particles. The model comprises of axial and radial dispersion, interfacial mass and heat transfer, nonlinear adsorption, and rectangular pulse injection. Also, a nonlinear system of partial differential equations coupled with differential and algebraic equations. An extended version of a semi-discrete high-resolution finite volume scheme (HR-FVS) is applied to approximate the model equations. Several case studies involving single- and multi-component elution are conducted to investigate the effects of key parameters, including the core radius fraction, adsorption enthalpy, axial and radial dispersion coefficients, equilibrium constants, and film mass and heat transfer coefficients. A standard performance metric is employed to assess the impact of thermal effects on process efficiency and to determine the optimal inert core radius. The results offer valuable insights for enhancing liquid chromatography systems under non-isothermal conditions with core-shell particles.

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