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Analysis of linear reactive general rate model of liquid chromatography considering irreversible and reversible reactions

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Abstract

A linear general rate model of two-component liquid chromatography is analyzed considering heterogenous reactions of types A→B and A⇄B. The model equations incorporate axial dispersion, external and intra particle pore diffusions, interfacial mass transfer, linear sorption kinetics, and first order heterogeneous chemical reactions. The solution methodology successively employs the Laplace transform and linear transformation steps to uncouple the governing set of coupled differential equations. The resulting system of uncoupled ODEs is solved by applying an elementary solution technique. The numerical Laplace inversion is employed to transform back the solutions in the actual time domain. The current solutions extend and generalize the recent solutions of nonreactive general rate model for single-solute transport. For validation, a high resolution finite volume scheme is implemented to obtain the numerical solutions. Different case studies are considered to verify the correctness of semi-analytical solutions and the accuracy of the numerical scheme. To further study the behavior of a chromatographic reactor, numerical temporal moments of the elution profiles are presented for both reactant and product. The derived semi-analytical solutions are useful tools to study the influence of solid phase reaction rate constant, interfacial mass transfer rate, intra particle pore diffusion, and reactant adsorption affinity on the concentration profiles.

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