



Linearly implicit-explicit schemes for the equilibrium dispersive model of chromatography



Raimund Bürger^{a,*}, Pep Mulet^b, Lihki Rubio^a, Mauricio Sepúlveda^a

^a *CI²MA & Departamento de Ingeniería Matemática, Universidad de Concepción, Casilla 160-C, Concepción, Chile*

^b *Departament de Matemàtiques, Universitat de València, Av. Dr. Moliner 50, E-46100 Burjassot, Spain*

ARTICLE INFO

Keywords:

Chromatography
Equilibrium dispersive model
Convection-diffusion equation
Implicit-explicit methods

ABSTRACT

Numerical schemes for the nonlinear equilibrium dispersive (ED) model for chromatographic processes with adsorption isotherms of Langmuir type are proposed. This model consists of a system of nonlinear, convection-dominated partial differential equations. The nonlinear convection gives rise to sharp moving transitions between concentrations of different solute components. This property calls for numerical methods with shock capturing capabilities. Based on results by Donat, Guerrero and Mulet (Appl. Numer. Math. 123 (2018) 22–42), conservative shock capturing numerical schemes can be designed for this chromatography model. Since explicit schemes for diffusion problems can pose severe stability restrictions on the time step, the novel schemes treat diffusion implicitly and convection explicitly. To avoid the need to solve the nonlinear systems appearing in the implicit treatment of the nonlinear diffusion, second-order linearly implicit-explicit Runge–Kutta schemes (LIMEX-RK schemes) are employed. Numerical experiments demonstrate that the schemes produce accurate numerical solutions with the same stability restrictions as in the purely hyperbolic case.

© 2017 Elsevier Inc. All rights reserved.

1. Introduction

1.1. Scope

Chromatography is used to separate complex fluid mixtures when a high purity of the product is demanded. In liquid batch chromatography, a pulse of fluid mixture, the solute, is injected at one end of a long cylindrical column filled with a porous medium (the stationary phase), followed by a continuous flow of liquid, the mobile phase, along the column. The solute interacts with the porous medium and its components begin to separate according to the strength of their affinity with the stationary phase. If the column is long enough, band profiles of single components move through it, so making it possible to collect pure fractions of components at its end.

The equilibrium dispersive (ED) model [14,19,25] is applicable when the mass transfer kinetics between the mobile phase and the stationary phase is fast, and when all band-broadening effects can be lumped into an apparent dispersion coefficient D_a . Within the ED model, chromatographic processes can be modeled by first-order nonlinear convection-dominated

* Corresponding author.

E-mail addresses: rburger@ing-mat.udec.cl (R. Bürger), mulet@uv.es (P. Mulet), lrubio@ing-mat.udec.cl (L. Rubio), mauricio@ing-mat.udec.cl (M. Sepúlveda).

conservation laws [14,22,23], coupled with some algebraic relations between the concentrations of the components of the mixture in the mobile and solid phases. Since analytical solutions can seldom be obtained, it is crucial to design numerical schemes for performing simulations with these models, and thereby to help practitioners to reduce the need for costly empirical experimentation.

There are other approaches that take into account the kinetics between the mobile phase and the stationary phase assuming that the equilibrium is not instantaneous, obtaining systems of equations with relaxation terms [15,16] (see also [14] for a more physical description). Both models (ED and relaxation) are similar when this relaxation parameter tends to zero.

Nonlinear convection terms cause sharp moving transitions between concentrations of different solute components and numerical methods should be able to cope with this situation, i.e., be conservative. Several works of simulation in chromatography propose conservative numerical schemes in which if D_a is null, then the roles of time t and of position z can be interchanged, being then the amounts conserved given by concentration in the mobile phase, and the flux given by the total solute concentrations (see [14,24]). These schemes are efficient and even used to solve certain problems of identification of parameters in chromatography [18] since they do not require the inversion of the nonlinear function that algebraically connects these two concentration vectors (total concentration and mobile phase concentration). The problem with these schemes is that, on the one hand, they do not conserve the original quantities, i.e., the total concentrations, and on the other hand, they cannot be applied if $D_a > 0$. In this sense it is proposed in [19] to suitably rewrite the model including the diffusion term and to solve it numerically by a non-conservative, linearized scheme in order to obtain an efficient method. However, Donat et al. [9] show that the non-conservative scheme proposed by Javeed et al. [19] for the simulation of the ED model can yield simulations for which the chromatographic fronts, that correspond to shocks when diffusion is neglected, move at a wrong speed and individual solute concentrations are not conserved when they should.

The main difficulty in the design of conservative numerical schemes in this formulation is that the conversion from conserved variables to primitive variables (concentrations of solute and mobile phases) can only be achieved through an implicit function whose properties can be deduced from the mathematical structure of the adsorption isotherm. Nevertheless this implicit function can be approximated numerically by efficient root finders.

The particular structure of the ED model [9], summarized in the next section, provides the theoretical background to implement conservative spatial semi-discretizations of the ED model (1.2), in a method of lines strategy. It is the purpose of this paper to advance fully discrete conservative numerical schemes that are obtained by applying suitable time integrators to the spatial semi-discretization. Explicit schemes applied to diffusion problems can strongly restrict the time step due to stability constraints. Therefore we aim to treat diffusion implicitly and convection explicitly. To avoid the necessity to solve nonlinear systems appearing in the implicit treatment of the nonlinear diffusion [6], we propose second-order linearly implicit-explicit Runge–Kutta schemes (in short, “LIMEX-RK” schemes) recently introduced in [1]. The same approach for the same purpose was proposed to handle similar problems in [3,4].

1.2. The equilibrium dispersive (ED) model of chromatography

We denote time by t and let z be the axial coordinate along the column that is normalized to have unit height, so that the top is at $z = 0$ and the bottom at $z = 1$. We assume that ε is the constant total porosity of the solid phase, i.e., the proportion of void space that can be occupied by fluid and u is the (constant) velocity of the mobile phase.

We denote by c_i the concentrations of the i th liquid phase and by q_i the concentration of solid phase adsorbent permeated by the i th phase. Thus, the total amount of liquid/solid material occupied by the i th phase is $\varepsilon c_i + (1 - \varepsilon)q_i$. The flux for the i th phase is postulated as $\varepsilon(u c_i - D_a \partial c_i / \partial z)$, so that the continuity equations of the ED model can be written as

$$\frac{\partial}{\partial t} (\varepsilon c_i + (1 - \varepsilon)q_i) + \frac{\partial}{\partial z} \left(\varepsilon \left(u c_i - D_a \frac{\partial c_i}{\partial z} \right) \right) = 0, \quad i = 1, \dots, N. \tag{1.1}$$

We assume that the mobile phase corresponds to the last index N . With the notation $\mathbf{c} := (c_1, \dots, c_N)^T$ and $\mathbf{q} := (q_1, \dots, q_N)^T$ and dividing (1.1) by ε , we obtain the system of continuity equations in the form

$$\frac{\partial}{\partial t} \left(\mathbf{c} + \frac{1 - \varepsilon}{\varepsilon} \mathbf{q} \right) + u \frac{\partial \mathbf{c}}{\partial z} = D_a \frac{\partial^2 \mathbf{c}}{\partial z^2}. \tag{1.2}$$

Appropriate boundary conditions for this model are proposed in [14], namely

$$u \mathbf{c} - D_a \frac{\partial \mathbf{c}}{\partial z} \Big|_{z=0} = u \mathbf{c}_{\text{inj}}(t), \quad \frac{\partial \mathbf{c}}{\partial z} \Big|_{z=1} = 0, \tag{1.3}$$

for a known function $\mathbf{c}_{\text{inj}}(t)$ that models the continuous injection of the liquid phases (components 1 to $N - 1$) and the “displacer” (component N) through the top of the column.

Within the ED model, the equilibrium relationship between the solid phase and liquid phase concentrations is given by the adsorption isotherm $\mathbf{q} = \mathbf{q}(\mathbf{c})$, which is usually a nonlinear function [14]. In this paper we consider multi-component mixtures for which the adsorption isotherms are of Langmuir type, that is

$$q_i = \frac{\alpha_i c_i}{1 + \beta^T \mathbf{c}}, \quad i = 1, \dots, N, \tag{1.4}$$

Download English Version:

<https://daneshyari.com/en/article/5775531>

Download Persian Version:

<https://daneshyari.com/article/5775531>

[Daneshyari.com](https://daneshyari.com)