



Implicit–Explicit WENO scheme for the equilibrium dispersive model of chromatography



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ABSTRACT

Chromatographic processes can be modeled by nonlinear, convection-dominated partial differential equations, together with nonlinear relations: the *adsorption isotherms*. In this paper we consider the nonlinear *equilibrium dispersive* (ED) model with adsorption isotherms of *Langmuir type*. We show that, in this case, the ED model can be written as a system of conservation laws when the dispersion coefficient vanishes. We also show that the function that relates the conserved variables and the physically observed concentrations of the components in the mixture is one to one and it admits a global inverse, which cannot be given explicitly, but can be adequately computed.

As a result, fully conservative numerical schemes can be designed for the ED model in chromatography. We propose a Weighted-Essentially-non-Oscillatory second order IMEX scheme and describe the numerical issues involved in its application. Through a series of numerical experiments, we show that our scheme gives accurate numerical solutions which capture the sharp discontinuities present in the chromatographic fronts, with the same stability restrictions as in the purely hyperbolic case.

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1. Introduction

Chromatography is a powerful tool for the separation of complex mixtures. 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 is distributed between the liquid and solid phases, and the components of the mixture begin to separate according to the strength of their interaction with the stationary phase. For a sufficiently long column, band profiles of single component-concentration travel along the column and it is possible to collect pure fractions of components at the outlet of the device. These tools are used for difficult separation tasks when a high purity of the product is demanded, as it is often the case in the pharmaceutical industry.

It has been long recognized that chromatographic processes can be modeled by considering non-linear, convection-dominated partial differential equations [20,14], coupled with some algebraic relations between the concentrations of the components of the mixture in the mobile and solid phases. Under reasonable assumptions, such as negligible dispersion effects and transport resistances, these equations become systems of first order non-linear conservation laws. Understanding the mathematical theory of these systems can enlighten many of the engineering aspects [20], in particular the formation and evolution of shock waves, which are an essential ingredient in the formation of band profiles of pure components. In

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addition, and since analytical solutions can only be obtained in very simple situations, it is important to develop tools that are able to perform accurate numerical simulations using these models. As observed in [22], robust and reliable numerical techniques can help practitioners to reduce the need for costly trial-and-error empirical experimentation.

In this paper we concentrate on the *equilibrium-dispersive* (ED henceforth) model. This is an ideal model based on the following assumptions (see e.g. [15,14])

1. There is a permanent equilibrium between the solid and mobile phases at all positions in the column.
2. The compressibility of the mobile phase is negligible and there is no interaction between the solvent (carrier) and the solid phase.
3. The porous medium in the column is homogeneous. Then, the adsorption process is uniform in time and axial direction.
4. There are no radial concentration gradients in the column.
5. Only axial dispersion causes band broadening. The column efficiency is characterized by an apparent axial dispersion coefficient $D_a > 0$, related to the height of the column, L , the (constant) velocity of the mobile phase, u , and the number of theoretical plates N_t , see [14], through the following relation

$$D_a = \frac{Lu}{2N_t}.$$

6. Any additional factor that could influence the adsorption behavior (such as the temperature) is neglected.

The mass balance equation of the ED model involves the concentrations of the N components of the mixture in the mobile phase, $\mathbf{c} = (c_1, \dots, c_N)^T$, and the solid phase, $\mathbf{q} = (q_1, \dots, q_N)^T$, and takes the following form

$$\frac{\partial \mathbf{c}}{\partial t} + \frac{1 - \epsilon}{\epsilon} \frac{\partial \mathbf{q}}{\partial t} + u \frac{\partial \mathbf{c}}{\partial z} = D_a \frac{\partial^2 \mathbf{c}}{\partial z^2} \tag{1}$$

where ϵ is the total porosity of the solid phase, $0 < \epsilon \leq 1$, t is the time and z 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 $z = 1$. Under the assumptions listed above, 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 non-linear function [14]. Appropriate boundary conditions for this model are proposed in [14]:

$$u\mathbf{c} - D_a \frac{\partial \mathbf{c}}{\partial z} \Big|_{z=0} = u\mathbf{c}_{inj}(t), \quad \frac{\partial \mathbf{c}}{\partial z} \Big|_{z=1} = 0, \tag{2}$$

for a known function $c_{inj}(t)$.

The form of the adsorption isotherm determines the mathematical structure of the solutions to the ED model. When dispersion is negligible, the model equations (1) and the algebraic relation $\mathbf{q} = \mathbf{q}(\mathbf{c})$ form a system of nonlinear, first order partial differential equations. The mathematical structure of the model for $N = 1$, i.e. *single-component* chromatographic elution, has been described in [20] for various types of adsorption isotherms.

In this paper we consider multi-component mixtures for which the adsorption isotherms are of *Langmuir type*, that is

$$q_i = \frac{a_i c_i}{1 + \sum_{i=1}^N b_i c_i}, \quad i = 1, 2, \dots, N, \tag{3}$$

where $a_i > 0$ are the Henry coefficients, and the coefficients $b_i > 0$ quantify the nonlinearity of the isotherm. For $N = 1$ and $D_a = 0$, the analysis of the resulting hyperbolic conservation law carried out in [20] shows that the solutions are characterized by continuous or discontinuous composition fronts that propagate along the separation unit. For $0 < D_a \ll 1$, (1) becomes a parabolic, convection-dominated PDE whose solutions may display very sharp fronts. The mathematical theory for the multi-component case seems to be much less developed.

Numerical simulations involving the nonlinear system (1) require efficient numerical techniques that can accurately describe discontinuous fronts. As reported by various authors (see e.g., [15] and references therein), finite element (FE) methods, normally used for diffusion dominated problems, often lead to numerical oscillations in convection-dominated problems whose solutions display sharp gradients, and it is also well known that spurious numerical oscillations are also observed when classical finite difference schemes (FD) are used for such problems.

In [15], the ED model (1)–(3) is rewritten as

$$\frac{\partial \mathbf{w}}{\partial t} + \frac{\partial(u\mathbf{c})}{\partial z} = D_a \frac{\partial^2 \mathbf{c}}{\partial z^2}, \quad \mathbf{w} = \mathbf{W}(\mathbf{c}) = \mathbf{c} + \frac{1 - \epsilon}{\epsilon} \mathbf{q}(\mathbf{c}) \tag{4}$$

and the authors propose to use a *conservative* discretization of the convective terms, $\partial_z(u\mathbf{c})$, combined with a standard centered discretization of the parabolic terms, in a finite volume (FV) framework. This numerical technique relies on the *understanding* that there is a one to one correspondence between the variables \mathbf{w} and the concentrations \mathbf{c} , so that (4) becomes a system of conservation laws when $D_a = 0$. Then, a *conservative discretization* of the convective terms guarantees mass conservation for the *conserved variables*, \mathbf{w} , and, as a consequence, the *shock-capturing* property, i.e. shocks (for $D_a = 0$)

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