NUMERICAL APPROXIMATIONS OF CHROMATOGRAPHIC MODELS

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Abstract. A numerical scheme based on modified method of characteristics with adjusted advection (MMOCAA) is proposed to approximate the solution of the system liquid chromatography with multi components case. For the case of one component, the method preserves the mass. Various examples and computational tests numerically verify the accuracy and efficiency of the approach.

Keywords: Advection-Diffusion, Coupled system, Langmuir adsorption model, Liquid Chromatography, Numerical approximation.

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1. INTRODUCTION AND PROBLEM SETTING

Chromatography is a technical process to separate mixed chemical components with a wide range of chemical industrial applications such as in pharmaceutical, food ingredients, etc. Here, we briefly explain the separation of components by liquid chromatography. In column chromatography a mixed sample is injected into a fluid stream which is called mobile phase. Then the fluid is pumped through a pipe which we refer as chromatographic column. The column is filled with very small porous beads called stationary phase. Different components in fluid adsorbs and/or desorbs at different rates on the stationary phase so they move through the column at different speeds and exit the column at different times; elution, see [6,9].

The transport of solutes in heterogeneous porous media is described by mass balance equation. The transport is influenced by the convection, diffusion, dispersion and also reaction/adsorption between solute and the porous environment. The model consists of system of convection-diffusion-reaction partial differential equations with dominating the convective terms coupled via differential or algebraic equations. To see different models and numerical approach, we refer to [9].

2. PRELIMINARIES AND PROBLEM SETTING

In one-dimension, the transport is given by the following coupled equations:

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\[
\begin{cases}
\frac{\partial u_i}{\partial t} + F \frac{\partial q_i}{\partial t} + v \frac{\partial u_i}{\partial x} = D \frac{\partial^2 u_i}{\partial x^2} & \text{in } (0, L) \times (0, T), \\
u_i(x = 0, t) = g_i(t) & \text{on } (0, T), \\
u_i(x, t = 0) = u_{i,0}(x) & \text{in } (0, L), \\
\frac{\partial u_i(x=L,t)}{\partial x} = 0 & \text{for } t \geq 0,
\end{cases}
\]

(2.1)

where,

- \( L \): the column length,
- \( t \): time,
- \( u_i \): concentration of the \( i \)-th component in the mobile phase,
- \( q_i \): concentration of the \( i \)-th component in the stationary phase,
- \( u_{i,0} \): initial condition,
- \( g_i \): boundary condition (injection profile),
- \( F \): stationary/mobile phase ratio,
- \( v \): mobile phase velocity,
- \( D \): diffusion parameter,
- \( m \): number of mixture components in the sample.

The Neumann boundary condition \( \frac{\partial u_i(x=L,t)}{\partial x} = 0 \) persuade continuity of the outlet concentration profile to the connecting tube receiving the fluid after leaving the column. The dispersion coefficient \( D \) is given by

\[
D = \frac{Lv}{2N_t},
\]

where \( N_t \) is the number of theoretical plates. The term \( F \) is given by

\[
F = \frac{1 - \epsilon}{\epsilon},
\]

which indicates the phase ratio based on the porosity \( \epsilon \). Also \( q_i \) is called adsorption isotherm and we assume that \( q_i = q_i(u_1, \ldots, u_m) \). In Langmuir model this term is given by

\[
q_i = \frac{a_i u_i}{1 + \sum_{j=1}^m b_j u_j}, \quad i = 1, 2, \ldots, m,
\]

(2.2)

where \( a_i, b_i > 0 \).

Let assume that the mass of components at the initial time in column is zero; \( u_{i,0}(x) = 0, \ 0 < x < L \). We consider rectangular injection profiles so boundary condition at the inlet point is:

\[
u_i(x = 0, t) = g_i(t) = u_{i,\text{inj}}(t),
\]

with

\[
u_{i,\text{inj}}(t) = \begin{cases} u_{i,f}(t) & 0 < t \leq t_{\text{inj}}, \\ 0 & t > t_{\text{inj}}, \end{cases}
\]

(2.3)
where \( u_i,f(t) \) is the inlet feed concentration and \( t_{inj} \) is the injection time. One can consider Danckwerts-type boundary conditions at the column inlet which is given by,

\[
u_i(x = 0, t) = u_{i,inj}(t) + \frac{D}{v} \frac{\partial u_i}{\partial x} \quad i = 1, \cdots, m,
\]

where for \( N_t > 100 \), e.g. Seidel-Morgenstern [20], it reduces again to

\[
u_i(x = 0, t) = u_{i,inj}(t).
\]

It is well known that in the convection dominate problems, discontinuity propagates in time even with the smooth initial and boundary data. Furthermore, the nonlinearity and coupling in term \( q_i \) in (2.1) brings more challenges to the numerical solution of this type of nonlinear coupled convection-diffusion system.

Standard finite difference, finite volume, and finite element methods are not stable and the numerical approximations exhibit non-physical oscillations and/or generates artificial numerical diffusion, which smear out sharp fronts of the solution [7,8,16].

In the case of scalar equation, one approach to eliminate the nonphysical oscillation which occurs on standard finite element or finite difference approach, is based on characteristic method. The sketch of idea is splitting the equation into two sub-steps, the convection step, which is solved explicitly by high order schemes (Lax Wendroff for instance), and the diffusion step, which is solved implicitly by central difference, see [1,3].

For the system (2.1), different approaches have been discussed. In [10] high resolution semi-discrete flux-limiting finite volume scheme is proposed which is capable to defeat numerical oscillations and preserves the positivity of numerical solution. The authors validate their scheme against other flux-limiting schemes available in the literature. To see about discontinuous Galerkin approximation for system (2.1) we refer to [11, 14, 15]. Recently in [19] a transport model is used to describe gradient elution in liquid chromatography. Furthermore, the authors implement Laplace transform to obtain the analytical solution of model.

In [2] the existence of the unique weak solution has shown for the case that \( q = \nabla \phi \) for some \( \phi : \mathbb{R}^m \to \mathbb{R} \), i.e the vector field \( q : \mathbb{R}^m \to \mathbb{R}^m \) in (2.1) can be expressed as a gradient of some non-negative \( C^1 \)-convex function \( \phi \). The proof is based on Rothe’s method along with solving a convex minimization problem at each time step which gives a numerical method to solve the coupled system.

We propose the modified method of characteristics with adjusted advection (MMOCAA) to solve the system of equation (2.1). This method was proposed by Douglas et al. to solve advection dominate transport PDEs [3]. The MMOCAA corrects the mass error occurs in the modified method of characteristic (MMOC) by perturbing the foot of the characteristics vaguely [4,17]. Our method is straight forward to implement and robust comparing the other methods mentioned above. Error analysis for presented scheme is beyond our aim in the current work.

The paper is organized as follows. Section 2 deals with introducing problem and previous works. In Section 3 we present our numerical scheme for
The iterative methods in (3.3) and (3.4) can be reformulated as

\[
\frac{\partial u_i}{\partial t} + F \frac{\partial u_i}{\partial x} + v \frac{\partial u_i}{\partial x} = D \frac{\partial^2 u_i}{\partial x^2} \quad \text{in } (0, L) \times (0, T),
\]

\[
\frac{\partial u_i}{\partial t} + F \frac{\partial u_i}{\partial x} + v \frac{\partial u_i}{\partial x} = D \frac{\partial^2 u_i}{\partial x^2} \quad \text{in } (0, L) \times (0, T),
\]

\[
(3.1)
\]

\[
u_k(x = 0, t) = g_i(t), \quad k = 1, 2 \quad \text{on } (0, T),
\]

\[
u_k(x, t = 0) = 0, \quad k = 1, 2 \quad \text{in } (0, L),
\]

\[
\frac{\partial u_i(x = L, t)}{\partial x} = 0, \quad \frac{\partial u_i(x = L, t)}{\partial x} = 0 \quad \text{for } t \geq 0.
\]

For the sake of simplicity, let’s assume that the number of components is two \((m = 2)\) however, it can simply extended for \(m > 2\).

\[
\begin{align*}
\frac{\partial u_i}{\partial t} + F \frac{\partial u_i}{\partial x} + v \frac{\partial u_i}{\partial x} &= D \frac{\partial^2 u_i}{\partial x^2} \quad \text{in } (0, L) \times (0, T), \\
\frac{\partial u_i}{\partial t} + F \frac{\partial u_i}{\partial x} + v \frac{\partial u_i}{\partial x} &= D \frac{\partial^2 u_i}{\partial x^2} \quad \text{in } (0, L) \times (0, T), \\
\text{for } k = 1, 2.
\end{align*}
\]

where \(\frac{\partial}{\partial x} \triangleq \frac{\partial}{\partial x} + v \frac{\partial}{\partial t}\) and \(v \frac{\partial}{\partial t} < 1\), the foot of backward characteristic \(\tilde{x}_i\) intersects \(t = t^n\) inside the interval \((x_{i-1}, x_{i+1})\). We can use quadratic interpolation between \(u_i^n, u_i^{n+1}, u_i^{n+1}\) which leads to the Lax-Wendrof scheme in the scalar case.

By method of characteristic we have

\[
u_k(x_i, t^{n+1}) = \tilde{u}_k^n(\tilde{x}_i) := u_k^n(x_i - v \Delta t), \quad \text{for } k = 1, 2.
\]

As \(\tilde{x}_i\) may not be a grid point, \(\tilde{u}_k^n(\tilde{x}_i)\) is an interpolated value. For \(v \frac{\Delta t}{\Delta x} < 1\), the foot of backward characteristic \(\tilde{x}_i\) intersects \(t = t^n\) inside the interval \((x_{i-1}, x_{i+1})\). We can use quadratic interpolation between \(u_i^n, u_i^{n+1}, u_i^{n+1}\) which leads to the Lax-Wendrof scheme in the scalar case.

By using the chain rule, we have

\[
\frac{\partial q}{\partial t} = \frac{\partial q}{\partial u_1} \frac{\partial u_1}{\partial t} + \frac{\partial q}{\partial u_2} \frac{\partial u_2}{\partial t}.
\]

We use the notation \(u(\cdot, t^n) = u^n(\cdot)\). To update the values of \(u = (u_1, u_2)\) at the point \((x_i, t^{n+1})\), we follow backward in the direction of the characteristic line. The semi-discretization of (3.1) reads as follows

\[
\frac{u_i^{n+1} - u_i^n}{\Delta t} + F \frac{\partial u_1^n}{\partial u_1} \frac{u_i^{n+1} - u_i^n}{\Delta t} + F \frac{\partial u_1^n}{\partial u_2} \frac{u_i^{n+1} - u_i^n}{\Delta t} = D(u_1^{n+1})_{xx},
\]

\[
(3.3)
\]

\[
\frac{u_i^{n+1} - u_i^n}{\Delta t} + F \frac{\partial u_2^n}{\partial u_1} \frac{u_i^{n+1} - u_i^n}{\Delta t} + F \frac{\partial u_2^n}{\partial u_2} \frac{u_i^{n+1} - u_i^n}{\Delta t} = D(u_2^{n+1})_{xx}.
\]

\[
(3.4)
\]

The iterative methods in (3.3) and (3.4) can be reformulated as

\[
\frac{u_i^{n+1} - \tilde{u}_i^n}{\Delta t} + F A^n \frac{u_i^{n+1} - u_i^n}{\Delta t} = D u_i^{n+1},
\]

where

\[
A^n = D^n \text{ and } F A^n = D^n + \left(\begin{array}{c}
\frac{\partial u_1}{\partial x} + v \frac{\partial u_1}{\partial t}
\end{array}\right).
\]
Remark 3.1. One can easily derive the weak formulation and semi-discretized system and do simulation based on that.

\[
\langle u^n - \bar{u}^{n-1}, \phi \rangle + \langle \nabla q^n (u^n - u^{n-1}), \phi \rangle + \Delta t \langle \nabla u^n, \nabla \phi \rangle + \Delta t \langle \nabla u^n, \phi \rangle = \langle \Delta t \langle g(t^n, u^{n-1}), \phi \rangle, \phi \rangle.
\]

where

\[
u^n(x) := \begin{pmatrix} u^n_1(x) \\ u^n_2(x) \end{pmatrix}.
\]

3.1. Ideal model. In the ideal model, we assumes that axial dispersion is negligible i.e., \( D = 0 \) which means that the column has an infinite efficiency and the thermodynamic equilibrium is achieved instantaneously.
3.1.1. Numerical approach. We can use MMOCAA explained in the previous section for the ideal case, i.e., $D = 0$. Here, we present a different approach that can be used for one ideal component ($m = 1$), i.e.,

$$\frac{\partial u}{\partial t} + F \frac{\partial}{\partial t} \left( \frac{au}{1 + bu} \right) + v \frac{\partial u}{\partial x} = 0.$$ 

Consider the change of variable

$$w = u + \frac{F}{1 + bu}.$$ 

The idea is to obtain the approximation of $w$ at point $(x_i, t^{n+1})$. Then $u$ can be recovered as function of $w$ by the following equation

$$u = -\left( Fa + 1 - bw \right) + \sqrt{(Fa + 1 - bw)^2 + 4bw}.$$ 

By Taylor’s expansion we have

$$w(x_i, t^{n+1}) = w(x_i, t^n) + \Delta t w_t(x_i, t^n) + \frac{(\Delta t)^2}{2} w_{tt}(x_i, t^n) + O(\Delta t)^3.$$ 

Next we obtain approximation for $w_t(x_i, t^n)$ and $w_{tt}(x_i, t^n)$. To do so, equation (3.9) implies that:

$$w_t = (1 + \frac{Fa}{(1 + bu)^2}) u_t.$$ 

By taking derivative with respect to $t$ from

$$w_t = -vu_x$$

and under some regularity assumption we obtain:

$$w_{tt} = (-vu_t)_x = -v(u_t)_x.$$ 

From (3.11) one has

$$u_t = \frac{w_t}{1 + \frac{Fa}{(1 + bu)^2}} = -\frac{vu_x}{1 + \frac{Fa}{(1 + bu)^2}}.$$ 

Next we have

$$(u_t)_x = -v(\frac{u_x}{1 + \frac{Fa}{(1 + bu)^2}})_x = -\frac{vu_{xx}}{1 + \frac{Fa}{(1 + bu)^2}} = 2v \frac{Faba(1 + bu)u_x^2}{((1 + bu)^2 + Fa)^2}.$$ 

The recent relation yields

$$w_{tt} = \frac{v^2 u_{xx}}{1 + \frac{Fa}{(1 + bu)^2}} + 2v^2 \frac{Faba(1 + bu)u_x^2}{((1 + bu)^2 + Fa)^2}.$$ 

We can substitute $w_t$ and $w_{tt}$ in (3.10) to obtain approximations for $w(x_i, t^{n+1})$ as below:

$$w_i^{n+1} = w_i^n - \frac{v}{2} \frac{\Delta t}{\Delta x} \delta_x u_i^n + \frac{v^2}{2} \left( \frac{\Delta t}{\Delta x} \right)^2 \left( \frac{\delta_x^2 u_i^n}{1 + \frac{Fa}{(1 + bu)^2}} + \frac{2Faba(1 + bu)(\delta_x u_i^n)^2}{((1 + bu)^2 + Fa)^2} \right),$$

where $\delta_x$ is the first central difference operator, $\delta_x^2$ is the second central difference operator, and $\Delta t$ and $\Delta x$ are the mesh-spacing in $t$ and $x$, respectively. The $i$ and $n$ are space and time indices, and $u_i^n$ is the grid function such that $u_i^n = u(x_i, t_n)$.
4. Numerical implication

In this section our scheme is validated with different tests. For scalar equation there exist many approaches with different flux limiters: Koren, Von leer, superbee, Minmod, Mc. For more detail about this methods refer to [10].

Example 4.1. To obtain accuracy and compare with analytical solution we consider the linear adsorption \( q = au \). The analytical solution of this case with linear adsorption with the parameters given in table 1 is derived in [18].

Table 1. Simulation parameters for the linear case study

| parameters                  | Symbols | Values | unite |
|-----------------------------|---------|--------|-------|
| Column length               | \( L \) | 1      | cm    |
| Porosity                    | \( F \) | 1.5    | -     |
| Interstitial velocity       | \( v \) | 1      | cm/min|
| Henry’s constant            | \( a \) | 1      | -     |
| constant in adsorption      | \( b \) | 0      | L/mol |
| Initial concentration       | \( u_0 \) | 0     | mol/L |
| Feed concentration          | \( u_{inj} \) | 1    | mol/L |
| Injection time              | \( t_{inj} \) | 3    | min   |
| Simulation time             | \( t_{max} \) | 7    | min   |

Figure 1 shows both analytical solution and approximated solution with the numbers of spatial steps \( n_x = 100 \) and of temporal steps \( n_t = 400 \).

Table 2 gives a comparison of \( L^1 \)-error and CPU time of our method with discontinuous Galerkin finite element method (DG-FE) with linear basis functions in [10,11] and with high order basis function of order 8 from [14].
Table 2. The comparison of the method used in [14] with MMOCAA

| Method          | DOFs | $L^1$ error | CPU time(s) |
|-----------------|------|-------------|-------------|
| DG-FM(ord=1)    | 16,000 | $6 \times 10^{-6}$ | 8827        |
| DG-FM(ord=8)    | 90   | $6 \times 10^{-8}$ | 0.7         |
| MMOCAA          | 100  | $15 \times 10^{-1}$ | 0.11        |

Table 3. $L^1$-norm and cpu time for different $n_x$ and $n_t$.

| $n_x$ | $n_t$ | $L^1$ error | CPU time(s) |
|-------|-------|-------------|-------------|
| 50    | 200   | $3 \times 10^{-1}$ | 0.0703      |
| 100   | 400   | $0.15 \times 10^{-1}$ | 0.11        |
| 200   | 800   | $0.11 \times 10^{-1}$ | 0.42        |
| 400   | 1600  | $7 \times 10^{-2}$ | 2.96        |
| 800   | 3200  | $5 \times 10^{-2}$ | 17.64       |

The $L^1$-norm of error and CPU time are presented in Table 3.

**Example 4.2.** Here we consider the one component model with nonlinear isotherm given as

$$q(u) = \frac{u}{1 + u}.$$  

The injection time is 0.2 and a rectangular pulse of hight 1 g/l is injected at inlet. The length of column is 1cm, the velocity $v = 1$ cm/min, $\epsilon = .5.$ and $N_t = 250$. Figure 2 shows the numerical simulation at outlet, compare with [11].

**Figure 2.** Profile of solution $u$ at outlet $x = 1$.

We can calculate the mass injected at the inlet during simulation time. Next, we compute the value of mass passing throughout each points for the time of simulation. Figure 3 indicates that the mass is preserved.
Figure 3. The values of approximated solution at different points in column.

| Different methods  | $L^1$ error | CPU time (s) |
|--------------------|-------------|--------------|
| First order        | 0.1146      | 0.43         |
| Korren             | 0.0497      | 0.56         |
| Van Leer           | 0.0586      | 0.56         |
| Superbee           | 0.0582      | 0.88         |
| Minmod             | 0.0645      | 1.45         |
| MC                 | 0.580       | 0.62         |
| Our approximation  | 0.0014      | 1.5          |

Table 4. The comparison of the method used in [10] with our approximate solution for one component nonlinear problem.

Because there is no analytical solution for these equations as reference solution, we consider $n_x = 3000$ grid points and $n_t = 20000$. Compare the result with the one in [10]. The $L^1$ error and CPU time are recorded in Table 4. We compare the results for the case of $n_x = 50$ grid points.

Example 4.3. In this example, we compare our simulation with the test given in [14], section 4.22. The parameters are chosen from Table 5 with $N_t = 5000$. Here the number of components is two; $m = 2$, however, there is no limitation to simulate with even larger numbers of theoretical plates. Figure 4 depicts numerical approximation for two components at outlet $x = 1$. See Table 6 for $L^1$ error and cpu time.

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Table 5. Simulation parameters for the nonlinear case study

| Parameters                     | Symbols | Values | unite |
|-------------------------------|---------|--------|-------|
| Column length                 | $L$     | 1      | m     |
| Porosity                      | $\epsilon$ | 0.4   | -     |
| Interstitial velocity         | $v$     | 0.1    | m/s   |
| Henry’s constant              | $a_1, a_2$ | 0.5, 1 | -     |
| Constant in adsorption        | $b_1, b_2$ | 0.05, 0.1 | L/mol |
| Initial concentration         | $u_{1,0}, u_{2,0}$ | 0, 0 | mol/L |
| Feed concentration            | $c_{f1}, c_{f2}$ | 10, 10 | mol/L |

Figure 4. Approximate solution for two components at outlet during simulation time.

| Different methods | $L^1$ error | CPU time(s) |
|-------------------|-------------|-------------|
| DG-FM(ord=8)      | 0.009       | 4.6         |
| Our approximation | 0.05        | 2.3         |

Table 6. The comparison with DG-FM in [14]

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