ANALYSIS OF EQUILIBRIUM DISPERSCIVE MODEL OF LIQUID CHROMATOGRAPHY
CONSIDERING A QUADRATIC-TYPE ADSORPTION ISOTHERM

Jamil UR REHMAN \textsuperscript{a}, Adeel MUNEER \textsuperscript{b,*}, Shamsul QAMAR \textsuperscript{a}

\textsuperscript{a}Department of Mathematics, COMSATS University Islamabad, Pakistan
\textsuperscript{b}Chair of Applied Mathematics (Continuous Optimization), Friedrich-Alexander-Universität Erlangen-Nürnberg,
Cauerstraße 11, 91058 Erlangen, Germany

\textsuperscript{*}Corresponding author: adeel.muneer@fau.de (Adeel Muneer), Tel: +49(0)9131 85-67177;

A single-component equilibrium dispersive model (EDM) of liquid chromatography is solved analytically for a quadratic-type adsorption isotherm. The consideration of quadratic isotherm leads to a nonlinear advection-diffusion partial differential equation (PDE) that hinders the derivation of analytical solution. To overcome this difficulty, the Hopf-Cole and exponential transformation techniques are applied one after another to convert the given advection-diffusion PDE to a second-order linear diffusion equation. These transformations are applied under the assumption of small nonlinearity, or small volumes of injected concentrations, or both. Afterwards, the Fourier transform technique is applied to obtain the analytical solution of the resulting linear diffusion equation. For detailed analysis of the process, numerical temporal moments are obtained from the actual time domain solution. These moments are useful to observe the effects of transport parameters on the shape, height and spreading of the elution peak. A second-order accurate, high resolution semi-discrete finite volume scheme is also utilized to approximate the same model for nonlinear Langmuir isotherms. Analytical and numerical results are compared for different case studies to gain knowledge about the ranges of kinetic parameters for which our analytical results are applicable. The effects of various parameters on the mechanism are analyzed under typical operating conditions available in the liquid chromatography literature.

\textbf{Key words:} Single-solute elution, quadratic isotherm, Hopf-Cole transformation, analytical solutions, moment analysis, numerical solutions.

1 Introduction

Liquid chromatography is a technique of separating mixture components that is based on different adsorptivities of the components to a specific adsorbent which is fixed inside a chromatographic column. The simplest process is the column liquid chromatography which involves a single column charged with pulses of fedded sample (mixture). These injected sample is carried through the column by some liquid desorbent. While traveling through the column, the more adsorptive component of the sample is retained longer by the adsorbent and, thus, leaves the column after the less adsorptive components. This technique is widely used by various researchers in the fields of biology, chemistry, biochemistry, as well as in environmental and clinical sciences. Such a popularity is due to its exceptional success in solving one of the most important problem of the experimental chemist, the physical separation of mixtures components rapidly, completely, and rather inexpensively, even when complex compounds are involved at either laboratory or at large scales. Models based on advection-diffusion equations are widely used with tremendous success for describing such separation processes \cite{1,2}. Various chromatographic models have been developed in the literature to simulate chromatographic processes. The most famous of them are the general rate model, various kinetic
models, and the equilibrium dispersive model (EDM) [3-5]. For linear adsorption isotherm, the analytical solutions of models are widely available in the literature [5-10]. There is close correlation between the equilibrium isotherm of a solute in a chromatographic system and the elution profile of its high concentration bands [5,11-14]. Various systematic investigations have proved good agreement between the experimental band profiles and the profiles calculated from the equilibrium isotherms [13,15,16]. In all studied cases, the isotherms were convex upward. The Langmuir isotherm is also convex upward and has no inflexion point. Simple statistical thermodynamics describes that the general form of an isotherm equation should be the ratio of two polynomials of the same exponent [13,14,17]. The analytical solutions for fast equilibrium with axial dispersion and nonlinear isotherm have been attempted in [13]. The authors have derived approximate results with single boundary, no solution being obtained for diffuse rear boundary. Band shapes in nonlinear chromatography with axial dispersion are also investigated in [19]. Furthermore, to answer the question about the peak shape and retention equilibrium, the statistical moments are very useful. In the literature, moment analysis approach is widely analyzed by a number of researchers [5,7,20-30].

The goal of this paper is to analytically solve the single-component equilibrium dispersive model (EDM) utilizing a polynomial-type quadratic adsorption isotherm. The inclusion of this quadratic-type isotherm in the mass balance equation leads to a nonlinear advection-diffusion PDE like a viscous Burger equation. It is known that analytical solution of Burger’s equation can be derived by applying a method discovered independently by Eberhard Hopf (1950) and Julian Cole (1951). As our EDM equation has resemblance to Burger’s equation, both Hopf-Cole and exponential transformations are applied one after another to convert the given advection-diffusion EDM to a second order linear diffusion equation. These transformations are applied under the assumption of small nonlinearity, or small volumes of injected concentrations, or both. Afterwards, the Fourier transform technique is applied to obtain the analytical solution of the resulting linear diffusion equation. Due to the importance of moment analysis, numerical moments are also derived in this work because of the non-possibility of analytical moments. Lastly, the HR-FVS is extended to solve the nonlinear isothermal model of liquid chromatography for comparison and validation of our assumptions [7,31]. Several test problems of practical interest are conducted.

The paper is divided in different sections as follows: In Section 2, a single-component EDM along with quadratic-type isotherm is introduced. In Section 3, the analytical solution of the model is derived for a pulse of finite width by the means of Hopf-Cole transformation. Expressions for numerical temporal moments are given in Section 4. In Section 5, various case studies are carried out to interpret the effects of model parameters on the concentration profiles. Finally, conclusions are drawn in Section 6.

2 The nonlinear equilibrium dispersive model

Consider the combined transport mechanisms of advection and diffusion for a single-component solute along with the following basic assumptions:

i The chromatographic process is isothermal and the mobile phase is incompressible, which holds for the liquid chromatography.

ii The concentration gradients along the radial axis are neglected and band broadening is due to axial dispersion only.

iii The packing material of stationary phase are porous spherical particles of same size and the bed is isotropic and homogeneous.

iv There is no interaction between the solid (stationary) phase and solvent (mobile) phase.

v The flow rate is assumed to be independent of axial dispersion coefficient.
In the case of single-solute EDM, the equation of mass balance for the transport of solute in the bulk of fluid is given as

\[
\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial z} = D_z \frac{\partial^2 c}{\partial z^2} - F \frac{\partial q}{\partial t},
\]

(1)

where \( c \) and \( q \) denote the concentration of the mobile and adsorbed phases, respectively. Further, \( F = \frac{(1 - \epsilon)}{\epsilon} \) is the phase ratio in terms of the total porosity \( \epsilon \), \( u \) is the interstitial velocity, \( D_z \) represents the axial dispersion coefficient, while \( t \) and \( z \) represent the time and axial coordinates.

Moreover, the following dimensionless quantities are introduced to reduce the number of variables

\[
x = \frac{z}{L}, \quad \tau = \frac{ut}{L}, \quad Pe = \frac{Lu}{D_z},
\]

(2)

where \( L \) is the length of the column, \( Pe \) is the Peclet number for the concentration, and \( \tau \) is the mean retention time of non-retained component. On using Eq. (2) in (1), we get

\[
\frac{\partial c}{\partial \tau} + \frac{\partial c}{\partial x} = \frac{1}{Pe} \frac{\partial^2 c}{\partial x^2} - F \frac{\partial q}{\partial \tau},
\]

(3)

The simplest isotherm model used in adsorption studies is the first order Langmuir isotherm [5, 13, 14, 17]:

\[
q(c) = \frac{ac}{1 + bc}.
\]

(4)

Assuming a fast injection of the sample as a rectangular profile of height \( c_{\text{inj}} \) and width \( \tau_{\text{inj}} \) such that the product \( c_{\text{inj}}\tau_{\text{inj}} \) expresses the sample size. Thus, we have to set the initial condition as:

\[
c(x, 0) = \begin{cases} 
c_{\text{inj}}, & 0 < x \leq \tau_{\text{inj}}, \\
0, & \text{otherwise}, \end{cases}
\]

(5)

where the symbols \( \tau_{\text{inj}} = ut_{\text{inj}}/L \) stands for the dimensionless time of injections. The boundary conditions for a hypothetically infinite length column are expressed as

\[
c(0, t) = 0, \quad c(\infty, t) = 0.
\]

(6)

3 Quadratic isotherm and Hopf-Cole transformation

Assuming small changes in the concentration, we can expand the nonlinear Langmuir adsorption isotherm around a reference value \( c_0 \) by applying Taylor expansion up to second order:

\[
q(c) = q(c_0) + \frac{\partial q}{\partial c} \bigg|_{(c = c_0)} (c - c_0) + \frac{\partial^2 q}{\partial c^2} \bigg|_{(c = c_0)} \frac{(c - c_0)^2}{2!}.
\]

(7)

After some manipulations and simplifications, the above equation simplifies to:

\[
q(c) = \gamma_1 + \gamma_2 c + \gamma_3 c^2,
\]

(8)

where

\[
\gamma_1 = \frac{ab^2 c_0^3}{(1 + bc_0)^3}, \quad \gamma_2 = \frac{a + 3abc_0}{(1 + bc_0)^3}, \quad \gamma_3 = \frac{-ab}{(1 + bc_0)^3}.
\]

(9)
The assumed quadratic isotherm has an edge that it is concave to the adsorbed solute for positive $\gamma_3$, while concave to the concentration axis for negative $\gamma_3$, and becomes linear for $\gamma_3 = 0$. In order to approximate the highly curved isotherm without the use of higher order polynomial isotherms, the constant $\gamma_1$ has been used. Using Eq. (8) in (3), we get

$$R \frac{\partial c}{\partial \tau} - \frac{1}{1 + \lambda c} \frac{\partial c}{\partial x} = \frac{1}{(1 + \lambda c)Pe} \frac{\partial^2 c}{\partial x^2},$$

(10)

where $R = 1 + \gamma_2 F$ and $\lambda = \frac{2F\gamma_3}{R}$. Here, $\lambda$ is a leaning parameter. Assuming $|\lambda c| << 1$, and also the quadratic and high order powers of $\lambda c$ can be neglected. Thus, we get

$$(1 + \lambda c)^{-1} \approx 1 - \lambda c.$$  

(11)

Moreover, for larger Peclet number (e.g. $Pe >= 500$), we can assume that $\frac{\lambda c}{Pe} \approx 0$.

After simplification, Eq. (10) becomes

$$R \frac{\partial c}{\partial \tau} + (1 - \lambda c) \frac{\partial c}{\partial x} = \frac{1}{Pe} \frac{\partial^2 c}{\partial x^2}.$$  

(12)

As a next step, we introduce a well known Hopf-Cole transformation to eliminate the nonlinear advection term from Eq. (12). Let us define

$$c(x, \tau) = \frac{2}{\lambda Pe} \frac{\omega_x(x, \tau)}{\omega(x, \tau)}.$$  

(13)

After some simplifications, the new dependent variable $\omega$ can be expressed as

$$\omega(x, \tau) = \exp \left( \frac{\lambda Pe}{2} \int_{-\infty}^{x} c(y, \tau) dy \right).$$  

(14)

where $y$ is an auxiliary integration variable and $c(y, \tau)$ represent axial distribution of solute at $\tau$. According to Eq. (5), we have to set $c(y, 0) = c_{inj} \tau_{inj} \delta(y)$ with $\delta(y)$ being a Dirac pulse function. It is defined as

$$\delta(y) = \begin{cases} 0, & y < 0, \\ 1, & y > 0. \end{cases}$$  

(15)

Thus, Eq. (14) for $\tau = 0$ becomes

$$\omega(x, 0) = \exp \left( \frac{\lambda Pe}{2} \int_{-\infty}^{x} c_{inj} \tau_{inj} \delta(y) dy \right).$$  

(16)

By incorporating Eq. (13) in Eq. (12), the nonlinear advection-diffusion PDE in Eq. (12) reduces to the following linear advection-diffusion PDE:

$$R \frac{\partial \omega}{\partial \tau} + \frac{\partial \omega}{\partial x} = \frac{1}{Pe} \frac{\partial^2 \omega}{\partial x^2}.$$  

(17)

Now, we can simplify the above advection-diffusion equation by introducing another transformation containing a new dependent variable $\phi(x, \tau)$, that is

$$\omega(x, \tau) = \phi(x, \tau) \exp \left( \frac{Pe_{x}}{2} - \frac{Pe_{\tau}}{4R} \right).$$  

(18)

The above transformation converts the linear advection-diffusion in Eq. (17) to a linear diffusion equation of the form:

$$\frac{\partial \phi}{\partial \tau} = \frac{1}{Pe} \frac{\partial^2 \phi}{\partial x^2},$$  

(19)

where $\tilde{Pe} = RPe$. 

4
4 Analytical solution by Fourier transformation

The Fourier transformation is applied as a primary tool to derive analytical solutions of Eq. (19). It is defined as

$$F[\phi(x, \tau)] = \tilde{\phi}(k, \tau) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp(ikx)\phi(x, \tau)dx,$$  \hspace{1cm} (20)

where $\tilde{\phi}$ and $\phi$ shows the solution profiles in Fourier-transformed and actual-space domains, respectively. After applying Fourier transformation on Eq. (19) we get

$$\tilde{\phi}(k, \tau) = \tilde{\phi}(k, 0) \exp(-\tau \tilde{Pe}k^2),$$  \hspace{1cm} (21)

here, $\tilde{\phi}(k, 0)$ is constant of integration at $\tau = 0$. By taking Fourier inverse of Eq. (21) and using initial conditions (IC) of Eq. (16) we reached at

$$\phi(x, \tau) = \int_{-\infty}^{\infty} \phi(x', 0) \sqrt{\frac{\tilde{Pe}}{4\pi\tau}} \exp \left( \frac{-(x - x')^2}{4\tau/\tilde{Pe}} \right) dx'.$$  \hspace{1cm} (22)

Here, $x'$ is the auxiliary variable. By using Eq. (22) in Eq. (18), we get

$$\omega(x, \tau) = \int_{-\infty}^{\infty} \sqrt{\frac{\tilde{Pe}}{4\pi\tau}} \exp \left[ \left( \frac{-(x - x')^2}{4\tau/\tilde{Pe}} \right) + \frac{\lambda Pe}{2} \int_{-\infty}^{x'} c_{inj} \tau_{inj} \delta(y)dy \right] dx'.$$  \hspace{1cm} (23)

After some algebraic manipulations, we get the following simplified form of above equation:

$$\omega(\xi, \tau) = \int_{-\infty}^{\infty} \sqrt{\frac{\tilde{Pe}}{4\pi\tau}} \exp \left[ \left( \frac{-(\xi - x')^2}{4\tau/\tilde{Pe}} \right) + \frac{\lambda Pe}{2} \int_{-\infty}^{x'} c_{inj} \tau_{inj} \delta(y)dy \right] dx',$$  \hspace{1cm} (24)

where $\xi = x - \frac{\tau}{R}$. After inserting the above equation in Eq. (13) and performing some algebraic manipulations, we get the following simplified solution in term of the actual concentration $c(x, \tau)$:

$$c(\xi, \tau) = -\frac{1}{\lambda e} \frac{\xi}{\sqrt{\lambda Pe} \tau} \exp \left[ -\frac{1}{\lambda Pe} \int_{-\infty}^{x'} \delta(y)dy \right] \frac{\exp \left( \frac{(\xi - x')^2}{2(\tau/\tilde{Pe})} \right)}{\sqrt{2\pi(\tau/\tilde{Pe})}} + \frac{1}{\lambda Pe} \int_{-\infty}^{x'} c_{inj} \tau_{inj} \delta(y)dy.$$  \hspace{1cm} (25)

The integral terms in the above equation can be simplified by utilizing the definition of Dirac step function given in Eq. (15) and by introducing a new parameter $\beta = \frac{\lambda Pe}{2} c_{inj} \tau_{inj}$. After calculating the above four integrals, we finally obtain the analytical solution of the form

$$c(\xi, \tau) = -\frac{2}{\lambda e} \exp \left( -\frac{\xi^2}{4\tau/\tilde{Pe}} \right) + \frac{2}{\lambda e} \exp(\beta - \frac{\xi^2}{4\tau/\tilde{Pe}}) \sqrt{\frac{\pi}{\tilde{Pe}}} \exp \left( \frac{-\xi}{2\sqrt{(\tau/\tilde{Pe})}} \right) \exp \left( \frac{\xi}{2\sqrt{(\tau/\tilde{Pe})}} \right) \erfc \left( \frac{-\xi}{2\sqrt{(\tau/\tilde{Pe})}} \right) + \sqrt{\frac{\pi}{\tilde{Pe}}} \exp \left( \frac{\xi}{2\sqrt{(\tau/\tilde{Pe})}} \right) \erfc \left( \frac{\xi}{2\sqrt{(\tau/\tilde{Pe})}} \right),$$  \hspace{1cm} (26)

where $\erf$ denotes the error function and $\erfc$ is the complementary error function, i.e. $\erfc(\zeta) = 1 - \erf(\zeta)$. 

5
5 Moment Analysis

In this section, temporal moments are discussed which are useful for analyzing and estimating the behavior of band profiles. Such moments provide overall information about the adsorption equilibrium and kinetic data. In the case of quadratic and nonlinear isotherms, analytical expressions of temporal moments are not obtainable. Therefore, numerical moments are calculated by numerically integrating their concentration profiles.

Numerous groups have worked on higher moments of chromatographic peaks in the mid nineteenes. In 1965, Kubin [20] and Kučera [21] calculated the moment equations independently. Furthermore, Grushka [33, 34] and Boniface [35] have worked on temporal moments.

In this study, the first four temporal moments are considered. The zeroth moment gives information about peak areas and total mass and the first moment \( \mu_1 \) corresponds to retention time. The second \( \mu'_2 \), third \( \mu'_3 \), and fourth \( \mu'_4 \) central moments give the information about variance (spreading), skewness, and kurtosis of the profiles, respectively.

The formulas for the numerical temporal moments at the column outlet are given as

\[
\mu_0 = \frac{L}{u} \int_0^\infty c(x = 1, \tau) \tau \, d\tau, \quad (27)
\]

\[
\mu_n = \left( \frac{L}{u} \right)^n \frac{\int_0^\infty c(x = 1, \tau) \tau^n \, d\tau}{\int_0^\infty c(x = 1, \tau) \, d\tau}, \quad n = 1, 2, 3, \ldots. \quad (28)
\]

The normalized \( n \)-th temporal moments are expressed as

\[
\mu_n = \left( \frac{L}{u} \right)^n \frac{\int_0^\infty c(x = 1, \tau) \tau^n \, d\tau}{\int_0^\infty c(x = 1, \tau) \, d\tau}, \quad n = 1, 2, 3, \ldots. \quad (29)
\]

The \( n \)-th central moment are obtained as

\[
\mu'_n = \left( \frac{L}{u} \right)^n \frac{\int_0^\infty c(x = 1, \tau) (\tau - \mu_1)^n \, d\tau}{\int_0^\infty c(x = 1, \tau) \, d\tau}, \quad n = 2, 3, \ldots. \quad (30)
\]

The above formula will be used to calculate numerical moments for the concentration profiles generated by analytical and FVS solutions.

6 Discussion on numerical test problems

This section presents a few case studies to analyze the applicability range of our derived analytical results. In the test problems, regenerated systems, i.e. \( c_{\text{init}} = 0 \) mol/l, and pulse injections of concentration \( c_{\text{inj}} = 1 \) mol/l and duration \( t_{\text{rminj}} = 2 \) min are considered. The analytical solutions are compared with the numerical solutions which are obtained through high resolution finite volume scheme of Koren considering either fully nonlinear isotherm (c.f. Eq. (4)) or quadratic isotherm (c.f. Eqs. (6) and (10)) [36].

The numerical moments are obtained from the proposed finite volume scheme using the moments formulas mentioned above. The trapezoidal rule is applied to numerically approximate the integral terms of these equations. A comparison of linear and quadratic numerical moments for different values of nonlinearity coefficients and flow rates are given. The parameters used for comparison are listed in Table 1.

Effect of the non-linearity coefficient \( b \): Figure 1 shows the results for different values of nonlinearity coefficient, i.e. for \( b = 0, 0.2, 1, 2 \). For \( b = 0 \) both quadratic and Langmuir isotherms become linear (c.f. Eqs. (4) and (5)) and, hence, a good agreement can be seen between the analytical and numerical results. While, plots for other values of \( b \) show that the results for quadratic isotherm start deviating from the
Table 1: Used parameters in the considered test problems.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>$L$ [cm]</th>
<th>$a$ [-]</th>
<th>$b$ [l/mol]</th>
<th>$u$ [cm/min]</th>
<th>$\epsilon$ [-]</th>
<th>$D_z$ [cm$^2$/min]</th>
<th>$c_{\text{init}}$ [mol/l]</th>
<th>$c_{\text{inj}}$ [mol/l]</th>
<th>$c_0$ [mol/l]</th>
<th>$t_{\text{inj}}$ [min]</th>
</tr>
</thead>
<tbody>
<tr>
<td>values</td>
<td>10</td>
<td>1.5</td>
<td>0.5</td>
<td>1.2</td>
<td>0.4</td>
<td>0.02</td>
<td>0</td>
<td>1</td>
<td>0.0001</td>
<td>2.0</td>
</tr>
</tbody>
</table>

results for Langmuir isotherm with the increase in the value of nonlinearity coefficient $b$. As the nonlinearity coefficient increases, the adsorption front of the profile becomes sharper and the desorption fronts becomes tailed. The results obtained endorse the use of quadratic isotherm for moderate values of the nonlinearity coefficient.

**Figure 1:** Effects of non-linearity coefficient on concentration profile, where $Pe = 600$. Other parameters are given in Table 1.

**Effects of different model parameters:** In Figure 2 the effects of different model parameters are shown. Figure 2(a) displays the effect of nonlinearity coefficient on the solution profiles, and also the analytical and numerical results for quadratic isotherm are compared with each other. A good agreement in the results verify the correctness of our analytical solution and accuracy of the proposed numerical algorithm. Figure 2(b) demonstrates the effect of Peclet number (or axial dispersion coefficient) on the solution profiles. It can be seen that solutions are diffusive for small value of the Peclet number (or larger axial dispersion coefficient), while profiles are narrower and sharper for large value of the Peclet number (or smaller axial dispersion coefficient). Figure 2(c) shows the influence of injection time on the profiles. It can be seen
that profiles become wider on increasing the injection time or injection volume. In Figure 2(d), the plot of concentration profiles for different values of Henry’s constant are displayed. It can be seen that for larger value of $a$, the retention time and spreading of concentration profile increases. In Figure 2(e) the various effects of leaning parameter $\lambda$ are shown. It can be observed that when value of $\lambda$ approaches to zero the shape of peak gets very close to Gaussian distribution and for the positive value of $\lambda$ i.e. 0.5 peak of the profile is left tailed, where as it is right tailed for $-0.5$.

Figure 2: Effects of different model parameters on concentration profile at $b = 1$ l/mol. All parameters are given in Table 1.
Effect of the nonlinearity coefficient on first four moments: Figure 3 shows the first four numerical moments obtained for different values of the nonlinearity coefficient $b$. It can be seen that moments for quadratic and Langmuir isotherms deviate from each other for larger values of the nonlinearity coefficient. Thus, it is once again verified that our analytical results for quadratic isotherm are useful for moderate values of the nonlinearity coefficient.

![Figure 3: Temporal moments as functions of nonlinearity coefficient $b$. Other parameters are given in Table 1.](image)

Effects of interstitial velocity on first four moments: Figure 4 gives a comparison of first four moments obtained by using quadratic and Langmuir isotherms at different values of flow rates $u$, while keeping the nonlinearity coefficient fixed as $b = 0.5$ l/mol. It can be seen that only third moments, representing asymmetry of the profiles, are deviating from each other.

![Figure 4: Effects of interstitial velocity on first four moments.](image)
Figure 4: Temporal moments as functions of interstitial velocity at fixed $b = 0.5$ l/mol. Other parameters are given in Table 1.

7 Conclusion

A single-component liquid chromatography model, based on quadratic isotherm, was solved analytically by using Hopf-Cole, exponential, and Fourier transformation techniques. To gain confidence on the generated profiles of concentration, the model equations were also solved numerically by applying a high resolution finite volume scheme. It was found that a better agreement between analytical and numerical solutions occurs up to a sufficiently large value of the nonlinearity coefficient. Furthermore, to investigate about the effects of transport parameters on the elution profiles, numerical temporal moments were obtained. Such moments are useful to interpret and understand the behavior of profiles inside the fixed-bed column. This study provides a feasible procedure of analyzing the column overloading and to determine the experimental operating conditions which will provide the optimum production rate in preparative liquid chromatography considering moderate changes in the concentrations. The results obtained are very helpful for better understanding of the physicochemical processes involved in liquid chromatography.
8 Acknowledgment

Adeel Muneer was partially funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)—Project (ID) 416229255—SFB 1411.

Nomenclature

\[ \begin{align*}
    a & : \text{Henry's constant, } \text{[} \text{mole/m}^2 \text{]} \\
    t & : \text{Time coordinate, } \text{[} \text{min} \text{]} \\
    c_0 & : \text{Reference concentration, } \text{[} \text{mole/l} \text{]} \\
    \text{c}_{\text{inj}} & : \text{Inlet concentrations, } \text{[} \text{mole/l} \text{]} \\
    D_{z,j} & : \text{Axial Dispersion coefficient, } \text{[} \text{cm}^2/\text{min} \text{]} \\
    \epsilon & : \text{External porosity, } \text{[} \text{m} \text{]} \\
    F & : \text{Phase ratio, } \text{[} \text{ } \text{]} \\
    z & : \text{Axial coordinate, } \text{[} \text{m} \text{]} \\
    c_{\text{init}} & : \text{Initial concentrations, } \text{[} \text{mole/l} \text{]} \\
    u & : \text{Interstitial phase velocity, } \text{[} \text{cm/min} \text{]} \\
    Pe & : \text{Peclet number, } \text{[} \text{ } \text{]} \\
    L & : \text{Column length, } \text{[} \text{m} \text{]} \\
\end{align*} \]

References


Revised: 17.03.2021.
Accepted: 18.03.2021.