



Efficient simulation of a separation column with axial diffusion and mass transfer resistance

Joaquin Menacho*, Oriol Pou, Xavier Tomás, Eduard Serra, Rosa Nomen, Julià Sempere

IQS School of Engineering, Universitat Ramon Llull, Via Augusta, 390, 08017 Barcelona, Spain

ARTICLE INFO

Article history:

Received 11 May 2012

Received in revised form 4 March 2013

Accepted 7 March 2013

Available online 15 March 2013

Keywords:

SMB

Preparative chromatography

Simulation

Lagrangian finite differences

ABSTRACT

The optimization of simulated moving bed systems is a complex task, and one of the difficulties is the lack of simulation methods that are sufficiently accurate and fast to be incorporated in the optimization algorithms. This paper presents a simulation of an adsorption column with finite differences based on a Lagrangian approach. The results obtained with this integration method were compared to values reported in the literature; the comparison shows that the accuracy of the integration method is not lower than that obtained with published methods and that this integration method requires a much lower cost in computation time. Various simulations were compared with experimental data for injections of caffeine and sodium 2-naphthalenesulfonate and with published results for the separation of isomers of omeprazole. The effects of axial diffusion and resistance to mass transfer on the elution curves were studied, and the simulation results were compared with the known theoretical analytical solution for a linear isotherm.

© 2013 Elsevier Ltd. All rights reserved.

1. Introduction

Optimization of the working parameters of simulated moving bed (SMB) separators is still a challenging issue. Because SMB reaches a cyclic steady state (CSS), not a constant one, and because many variables are involved, this task is complex (Grosfils, Levrie, & Kinnaert, 2007; Kawajiri & Biegler, 2006; Kim, Lee, & Lee, 2010; Sempere et al., 2010). Nevertheless, this issue has recently been the subject of a wide variety of studies. Most of the studies are based on the analysis of the analogous true moving bed (TMB) system through the so-called “standing wave analysis” (Buhler, Lehr, & Jungbauer, 2009; Cauley, Cauley, & Wang, 2008; Djohari & Carr, 2005; Lee, Mun, Cauley, Cox, & Wang, 2006; Ma & Wang, 1997) or through “equilibrium theory” (Mazzotti, 2006a, 2006b, 2006c; Migliorini, Gentilini, Mazzotti, & Morbidelli, 1999; Sempere et al., 2008). These methods converge to an optimal theoretical solution (Cauley et al., 2004) based on an analysis of the velocities of the concentration fronts through the adsorption column. This analysis allows a set of working parameters at ideal conditions to be calculated rapidly, but the assumption of ideal conditions implies a lack of accuracy that depends on the importance of non-idealities in the system considered.

Optimization methods can be grouped into two families (Lübke, Seidel-Morgenstern, & Tobiska, 2007). One family consists of the

direct calculation of the CSS of the system after both space and time are discretized along an entire period and forces the displaced periodicity of the solution (Rodrigues, Silva, & Mota, 2010; Toumi, Engell, Diehl, Bock, & Schlöder, 2007). In contrast, direct methods consist of the sequential simulation of every column and include the corresponding material balances in the connecting nodes (Dünnebier and Klatt, 2000; Strube & Schmidt-Traub, 1998). This last perspective is a true simulation of the SMB and passes through all of the different transient states up to the CSS. This strategy also allows changes in working conditions to be simulated. The problem with this type of method is the computational cost of the sequential simulation, which is repeated until the CSS is reached each time the objective function is evaluated. The usual simulation techniques are often too time-consuming to allow such a strategy. Therefore, it is interesting to find new ways to perform such simulations.

The numerical techniques used most often to simulate adsorption and ion-exchange columns are the finite difference (FD) approach (Djohari & Carr, 2005; Ma & Guiochon, 1990), the method of lines (MoL) (Montesinos-Cisneros et al., 2010; Vande Wouwer, Sauter, & Schiesser, 2004) and the orthogonal collocation on finite elements (FE) approach (Asnin, Kaczmarski, & Guiochon, 2007; Kim et al., 2010; Lü, Wei, Shen, Ren, & Wu, 2006; Rodrigues et al., 2010; Toumi et al., 2007; Wang & Ching, 2003). The last method generally offers greater precision than the others, especially when the boundary conditions of the simulation are not easily achieved. This situation occurs when it is necessary to simulate the movement of “shock waves” of concentration in a system with high diffusion or

* Corresponding author. Tel.: +34 932 672 000.

E-mail address: joaquin.menacho@iqs.edu (J. Menacho).

Nomenclature

c	concentration in mobile phase
c_{inj}	concentration of the sample injected
D	axial diffusion coefficient
F	volume ratio $= (1 - \varepsilon)/\varepsilon$
k	mass transfer coefficient
L	column length
Pe	Péclet number
q	concentration in stationary phase
Q	volumetric flow
St	Stanton number
t_p	duration of injection pulse
u	interstitial velocity
w	concentration wave velocity
z	adimensional space
γ	adimensional concentration
ε	total void fraction
τ	adimensional time

mass transfer coefficients. However, this case is very often unavoidable in chromatographic columns. In numerical simulations, those characteristics easily cause numerical instability. Because of the steepness of the concentration profiles, the number of mesh points plays an important role in the accuracy of the solution and in the computation time. Avoiding instabilities usually requires smoothing the solution or using very narrow or adaptive meshes; these meshes imply a computation time that is too long. Alternatively, the average CSS concentrations of the extract and the raffinate of the SMB can be overestimated or underestimated because of a small number of mesh points (Lim & Jorgensen, 2004). Salgado and Aranda (2007) affirm that no integration method has yet succeeded in all cases (high and low mass resistance, and strong and weak diffusion) and that a compromise must be achieved between accuracy and computation time.

In previous work (Menacho et al., 2011), a method to solve the chromatographic model with mass transfer, but without diffusion effects, was studied. The low computational cost of the method was confirmed, especially when this cost was compared to that of orthogonal collocation on finite elements. The improvement was 60–90% in the studied cases.

The aim of this work is to test the performance of this numerical scheme when it is extended to simulate adsorption columns with mass transfer and axial diffusion effects; thereby achieving a good precision with a computation time low enough to allow use of the scheme in direct optimization. This method takes a perspective that converges with the method proposed by Salgado and Aranda (2007), which was formulated as an agent-based procedure. The method is based on changing the direction of the integration mesh for the fluid phase as a type of Lagrangian formulation on finite differences (LFD). The simulation results are compared to those obtained by the other usual methods, and this comparison establishes the precision and computational costs of this method. The simulations are also validated by comparing their results with data from experiments and from published literature.

2. Modeling

2.1. Mathematical model and integration scheme

There are several mathematical approaches to express the mass balance in a separation column, and these approaches depend on the hypothesis that is assumed. The simplest model is named the equilibrium ideal model; in this model, phase equilibrium is

assumed, and no diffusion occurs. The mass balance under these conditions is

$$\begin{cases} \frac{\partial c}{\partial t} + F \frac{\partial q}{\partial t} + u \frac{\partial c}{\partial x} = 0 \\ q = f(c) \end{cases} \quad (1)$$

where q and c are the concentrations of the species in the liquid and solid phases, respectively. F is the phase volume ratio, and $f(c)$ is the adsorption isotherm. Because:

$$\frac{\partial q}{\partial t} = \frac{\partial q}{\partial c} \times \frac{\partial c}{\partial t} = f'(c) \times \frac{\partial c}{\partial t} \quad (2)$$

The system of equations can be written

$$\begin{cases} \frac{\partial c}{\partial t} + \frac{u}{1 + F \times f'(c)} \times \frac{\partial c}{\partial x} = 0 \\ q_i = f(c_i) \end{cases} \quad (3)$$

The first equation is a simple wave propagation. A change of variables can be performed:

$$\begin{cases} r = x - wt \\ s = t \end{cases} \quad (4)$$

where $w = \frac{u}{1 + F \times f'(c)}$

Thus, the first equation becomes:

$$\frac{\partial c}{\partial s} = 0 \quad (5)$$

The solution is a function: $c(r, s) = \varphi(r)$

$$c(x, t) = \varphi(x - wt) \quad (6)$$

This solution means that the concentration is constant along the characteristic lines $x - wt = \text{constant}$ in the $x-t$ plane. Thus, the concentration profile along the column behaves similarly to a concentration wave that moves along the column with a velocity w . For linear isotherms, the velocity w is constant; therefore, the pulse injected at the inlet moves along the column at a constant speed and exits without a change in shape.

The solution of the equilibrium ideal model is interesting because more sophisticated and realistic models can be regarded as variations of this model that incorporate the effects of non-idealities.

The transport diffusion model (TDM) is a very usual non-ideal model; it assumes that there is a uniform concentration in the radial dimension, molecular diffusion in the axial direction, and mass transfer caused by a linear driving force

$$\begin{cases} \frac{\partial c_i}{\partial t} + F \frac{\partial q_i}{\partial t} + u \frac{\partial c_i}{\partial x} = D \frac{\partial^2 c_i}{\partial x^2} \\ \frac{\partial q_i}{\partial t} = k(q_{eq,i} - q_i) \end{cases} \quad (7)$$

where $q_{eq,i} = f_i(c_1, \dots, c_n)$ is the equilibrium concentration of the i th species in the stationary phase and depends directly on the isotherm, D and k are the diffusion and mass transfer effective coefficients, u is the interstitial velocity, and F is the phase volume ratio. The set of equations expresses the mass balance of both the mobile and stationary phases.

Inspired by the solution for the equilibrium ideal model, a change of coordinates for the first equation is proposed.

$$\begin{cases} r = x - ut \\ s = t \end{cases} \quad (8)$$

Download English Version:

<https://daneshyari.com/en/article/172619>

Download Persian Version:

<https://daneshyari.com/article/172619>

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