



On minimal representation of heterogeneous mass transfer for simulation and parameter estimation: Application to breakthrough curves exploitation

Françoise Couenne, Christian Jallut, Mélaz Tayakout-Fayolle*

Laboratoire d'Automatique et de Génie des Procédés, UMR CNRS 5007, Université Claude Bernard et Ecole Supérieure de Chimie, Physique-Electronique de Lyon, 43 BD du 11 Novembre 1918, 69622 Villeurbanne Cedex, France

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Abstract

This paper deals with the problem of mass transfer representation within heterogeneous systems. For the purpose of their modelling from material balances, it is emphasised the existence of a well-suited change of state variables which leads to a representation containing a minimal number of parameters. The benefits of the proposed approach are illustrated by an example of parameter estimation performed from experimental breakthrough curves in chromatography. Experimental data concerning the adsorption of p-nitrophenol onto granular activated carbon are taken from [Chern, J., Chien, Y. (2002). Adsorption of nitrophenol onto activated carbon: isotherms and breakthrough curves. *Water Research* 36, 647–655]. This representation has several advantages: from a numerical point of view for simulation and also for parameter estimation since the number of parameter groups (macro-parameters) is minimal. In order to confirm the relevance of the change of coordinates that we propose, a structural identifiability study is also performed in some cases.

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1. Introduction

Parameter estimation is extensively used in chemical engineering to determine transport properties, kinetics as well as thermodynamic equilibrium constants (Jallut, Thomas, Touré, & Diard, 2001). The treatment of experimental data obtained from chromatographic columns is a typical example of such an approach. This technique is used to characterise liquid or gas phase adsorbents (Golshan-Shirazi & Guiochon, 1992; Gritti, Piatkowski, & Guiochon, 2002; Hufton & Danner, 1993a, 1993b; Jolimaitre, Tayakout-Fayolle, Jallut, & Ragil, 2001; Tondeur, Kabir, Luo, & Granger, 1996), soils (Chen & Wagenet, 1995) as well as polymers (Von Meien, Biscaia, & Nobrega, 1997). One can perform specific experiments to extract the values of some of the parameters. For example, the frontal technique allows to determine the equilibrium isotherm by performing a global mass balance of the adsorbate (Gritti & Guiochon, 2003). Axial dispersion coefficient as well as porosities can be estimated from inert tracer experiments (Hejtmanek & Schneider, 1993). The other approach consists in performing the estimation of all the parameters from only one experiment. Such an approach allows to minimize the sources of errors, to save time and to avoid numerous experiments (Altenhöner, Meurer, Strube, & Schmidt-Traub, 1997). However, as far as the number of parameters to estimate is greater, a structural analysis of the model has to be performed.

In this paper, we propose a way to derive models for chromatographic columns in order to avoid a possible overparametrization and we link this question to the structural identifiability of the parameters. This approach is applied to distributed parameter models. We restrict ourselves to the case of a single component experiment: an adsorbate is transported isothermally by a carrier and is supposed to be adsorbed in a solid phase. When it is introduced according to a step function from an equilibrium state, the response

* Corresponding author. Tel.: +33 472431882

E-mail address: tayakout@lagep.univ-lyon1.fr (M. Tayakout-Fayolle).

Nomenclature

| | |
|-----------------------|---|
| $a_p = 3/R$ | pellet volumetric surface area ($\text{m}^2 \text{m}^{-3}$) |
| A, B | parameters for the Redlich–Peterson equilibrium model (mol m^{-3}) ^{M} |
| C_{f1} | adsorbate concentration in the mobile phase (mol m^{-3}) |
| C_{f1}^* | adsorbate concentration in a mobile phase at equilibrium with a solid (mol m^{-3}) |
| C_{in} | adsorbate inlet concentration (mol m^{-3}) |
| $f(), g(), \hat{f}()$ | vector fields |
| $g^{eq}() = 0$ | equilibrium relation (mol m^{-3}) |
| $h()$ | output equation |
| H | Hessian matrix |
| i | index for the CSTR or the sample time |
| $J(\theta)$ | criteria to minimize |
| k | number of parameters to be estimated |
| k_p, k'_p | equivalent mass transfer coefficient in the LDF model ($\text{m}^2 \text{s}^{-1}$) |
| k_1 | parameter for the Langmuir model |
| k_2 | parameter for the Langmuir model ($\text{m}^3 \text{mol}^{-1}$) |
| L | column length (m) |
| M | parameter for the Redlich–Peterson equilibrium model |
| N | number of CSTRs in the lumped parameters model |
| N_p | number of sample points |
| Pe | Peclet number |
| q | adsorbate concentration within the adsorbent (mol m^{-3}) |
| q_0 | initial adsorbate concentration within the adsorbent (mol m^{-3}) |
| q^* | adsorbate concentration within the adsorbent in equilibrium with a fluid phase (mol m^{-3}) |
| Q | volumetric flow rate through the column ($\text{m}^3 \text{s}^{-1}$) |
| R | pellet mean radius (m) |
| s | Student variable |
| S | sensitivity matrix |
| t | time (s) |
| u | input |
| v | interstitial fluid velocity (m s^{-1}) |
| x, x_0 | state space vector and its initial value |
| y_{mod} | simulated output |
| y_{meas} | simulated output |
| z | bed axial coordinate (m) |

Greek letters

| | |
|--|---|
| $\alpha, \beta, \gamma, \delta$ | notations for the parameters in Eq. (11) |
| ε_f | bed external porosity |
| θ, θ' | parameters vector |
| $\hat{\theta}$ | estimation of θ |
| $\xi = z/L$ | dimensionless axial coordinate |
| σ | variance |
| $\tau_1, \tau_p, \tau'_p, \tau_c, \tau'_c$ | mass transfer time constants involved in the models (s^{-1}) |

of the system is the breakthrough curve. The models that are used to extract parameters from experimental breakthrough curves are formulated in the state space from suitable material balances of the adsorbate, according to the general form (1):

$$\begin{cases} \dot{x} = \frac{\partial x}{\partial t} = f(x, u, \theta) \\ g^{eq}(x^*, x, \theta) = 0 \\ y(t) = h(x, u, \theta) \\ x(t = 0) = x_0(\theta) \end{cases} \quad (1)$$

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