



ELSEVIER

Journal of Chromatography A, 876 (2000) 3–15

JOURNAL OF
CHROMATOGRAPHY A

www.elsevier.com/locate/chroma

Design and optimisation of a simulated moving bed unit: role of deviations from equilibrium theory

Giovanni Biressi^a, Olivier Ludemann-Hombourger^b, Marco Mazzotti^c,
Roger-Marc Nicoud^b, Massimo Morbidelli^{a,*}

^aLaboratorium für Technische Chemie, ETH Zürich, CAB C40, Universitätstrasse 6, CH-8092 Zürich, Switzerland

^bNovasep SA, 15 Rue du Bois de la Champelle, Parc Technologique de Barbois, B.P. 50, F-54502 Vandœuvre-lès-Nancy, France

^cInstitut für Verfahrenstechnik, ETH Zürich, Sonneggstrasse 6, CH-8092 Zürich, Switzerland

Received 1 October 1999; received in revised form 25 January 2000; accepted 4 February 2000

Abstract

The design of a simulated moving bed involves thermodynamic, kinetic and hydrodynamic aspects and requires the optimisation of several variables: plant design variables, such as the column length and diameter, and operating variables, among them four independent flow-rates, the feed concentration and the switch time. In this work we develop an algorithm to design both the unit and its operating conditions, with an overall view on equilibrium properties, efficiency and hydrodynamics, using a simple equilibrium stage model. In this way we determine the parameters leading to the highest possible productivity for a given separation, only requiring the knowledge of the equilibrium isotherms, the Van Deemter equation and a correlation for pressure drop. The algorithm has been used to investigate the effect on the separation performance of some parameters, such as particle size and required product purity, which are not considered by equilibrium theory. The results have been compared with the predictions of equilibrium theory and the observed deviations have been put in evidence and discussed. © 2000 Elsevier Science B.V. All rights reserved.

Keywords: Simulated moving bed; Equilibrium theory; Preparative chromatography

1. Introduction

The simulated moving bed (SMB) is an important technique, introduced in the early 1960s by UOP for the large-scale separation of hydrocarbons (cf. the SORBEX process) [1,2]. Processes based on this technology were developed in the following years first in the sugar industry and later, in the early 1990s, for fine chemical separations [3–5]. Since

SMB is particularly suited for binary separations, it became the technology of choice for various chiral separations, as indicated for example by several high-performance liquid chromatography (HPLC)–SMB enantiomer separations recently studied in the literature [6–8]. Also biotechnological [9], gas chromatographic [10,11] and supercritical [12] SMB applications have been investigated.

All these applications have in common the fact of realising a continuous preparative chromatographic process, where the counter current contact between the fluid mixture and the selective packing material is simulated by periodically switching the inlet and

*Corresponding author. Tel.: +41-1-6323-034; fax: +41-1-6321-082.

E-mail address: morbidelli@tech.chem.ethz.ch (M. Morbidelli)

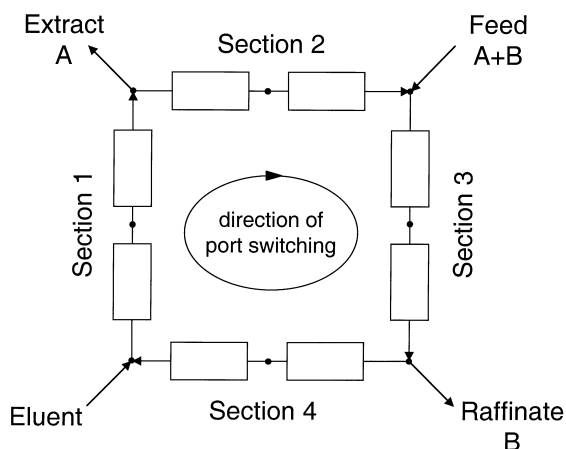


Fig. 1. Scheme of a SMB unit.

outlet ports of the plant in the same direction of the fluid motion, according to the scheme in Fig. 1. In this picture the most widely adopted scheme consisting of four sections is represented, but also two and three section units can be used [2,10]. Each section plays a specific role in the separation.

With reference to the scheme reported in Fig. 1, the separation is carried out in sections 2 and 3. In the case of a binary mixture the feed stream carries the two components to be separated in section 3. The least adsorbable component, B, is eluted from the column before the port switching takes place and therefore it exits the unit in the raffinate stream. Meanwhile the most adsorbable component, A, remains completely adsorbed on the solid phase and, as a consequence of port switching, it remains in the column until it reaches section 1, where it is eluted in the extract stream. With proper working conditions, A is not eluted from the columns of section 3 and B does not remain adsorbed in columns of section 2 at the end of the switching period, so it does not appear in section 1. In section 4, B is adsorbed on the columns, so the eluent is cleaned and can be recycled to section 1.

With SMBs high separation performances can be reached even with rather low selectivities and with a small number of theoretical plates [13]. This is due to the counter current contact and to the fact that, contrary to batch preparative chromatography, the peaks of the two products do not have to be completely separated all along the columns, but only

at the locations where the extract and the raffinate are withdrawn. Therefore, this technology is more and more applied to scale up analytical or small-scale batch preparative chromatographic separations, leading to a more efficient process with higher productivity and smaller eluent consumption.

In order to establish the economic feasibility of an SMB separation process, we need to use design methods that identify the optimal operating conditions as well as the required size of the unit involved. This work provides such a procedure, which we describe in the following with reference to simple SMB models. This procedure represents an improvement with respect to similar ones presented in the literature, which is especially significant in the case of non linear adsorption equilibria [13,14].

In particular, it must be noted that in the procedure by Charton and Nicoud [13] the optimal set of flow-rates according to equilibrium theory is simply used, while dispersion is considered only for calculating the column size. On the contrary, this new procedure is completely based on a detailed model and uses equilibrium theory's predictions only as a reference. This allows us to analyse how deviations from equilibrium theory affect the design of a new SMB unit, which is one of the main objectives of this work.

In the application of the design procedure described in the following, the SMB unit has been simulated using a steady state equilibrium stage model for a true moving bed (TMB) unit. The two unit configurations, SMB and TMB, achieve the same steady state separation performance when the following kinematic and geometric conversion rules are satisfied:

$$Q_j^{\text{TMB}} = Q_j^{\text{SMB}} - Q_s \cdot \frac{\epsilon_b}{1 - \epsilon_b} \quad (1)$$

$$Q_s = \frac{(1 - \epsilon_b)V}{t^*}$$

where Q_j^{SMB} and Q_j^{TMB} are the volumetric flow-rates in section j of the SMB and the TMB units, respectively, V is the volume of a column, t^* is the switch time in the SMB unit, Q_s is the solid flow-rate in the TMB unit and ϵ_b is the external porosity.

The unit is regarded as consisting of a series of several stages, where perfect mixing and adsorption

equilibrium conditions are assumed. The stages are connected by the fluid and solid counter current flows given by the conversion rules discussed above [13]. The number of stages in each section corresponds to the number of theoretical plates in the section and therefore characterises its efficiency. With this approach, the model simply consists of the mass balance equations for each stage:

$$Q_j^{\text{TMB}}(c_{i,n} - c_{i,n-1}) + Q_s \cdot [(1 - \epsilon_p) \cdot (q_{i,n} - q_{i,n+1}) + \epsilon_p \cdot (c_{i,n} - c_{i,n+1})] = 0 \quad (2)$$

where Q_j^{TMB} is the fluid volumetric flow-rate in section j of the TMB unit, Q_s is the solid volumetric flow-rate in the TMB unit, $c_{i,n}$ is the fluid concentration of the i -th component in the n -th stage, $q_{i,n}$ is the concentration of the i -th component on the solid in the n -th stage at equilibrium with the fluid phase and ϵ_p is the internal porosity of the packing material. This equation is based on the assumption that the fluid concentration in the bulk and in the pores of the solid phase is the same, since in each stage thermodynamic equilibrium is assumed and the case of size-exclusion chromatography is not considered.

2. The optimisation problem

To design an SMB we need to determine the column length and section that allow to achieve the desired purity in the outlet streams with the maximum specific productivity and without exceeding given pressure drop limits imposed by the packing material adopted. This can be obtained by properly optimising the unit operating conditions, which requires a proper characterisation of the thermodynamic, kinetic and fluid dynamic behaviour of the unit. In practice, a satisfactory result is obtained using three distinct pieces of information, the adsorption equilibrium isotherms, the Van Deemter equation and a correlation for the pressure drop.

In the following we will assume that the distribution of columns in each section as well as the feed concentration are fixed. In this case the SMB unit and its operating conditions are fully determined by seven independent variables including column length and section, flow-rates in the four sections of

the unit and switch time. For convenience we select the following set of design variables: the flow-rate in section 1 (Q_1^{SMB}), column length and section (L , Ω) and the flow-rate ratios in the four sections (m_1 , m_2 , m_3 , m_4), which are defined as:

$$m_j = \frac{Q_j^{\text{SMB}} t^* - V \epsilon^*}{V \cdot (1 - \epsilon^*)} \quad (3)$$

where ϵ^* is the total porosity, i.e., $\epsilon^* = \epsilon_b + (1 - \epsilon_b) \cdot \epsilon_p$.

The procedure we are going to describe enforces as optimisation constraints the maximum allowable pressure drop in each column and the minimum purity requirements for both, raffinate and extract streams. The optimisation objective is the specific productivity, defined as mass of racemate per unit time and volume of solid phase:

$$\text{prod}_V = \frac{Q_F c_{T,F}}{V_{\text{SP}}} = \frac{c_{T,F} \cdot (m_3 - m_2) \cdot (1 - \epsilon^*)}{t^* n_{\text{col}}} \quad (4)$$

where $c_{T,F}$ is the overall feed concentration, Q_F the feed volumetric flow-rate, V_{SP} the total volume of solid phase, n_{col} the number of columns in the unit.

3. The optimisation procedure

The main design equations, in addition to the countercurrent equilibrium stage model reported above, are a correlation for estimating pressure drop and the Van Deemter equation for the height equivalent to a theoretical plate HETP_{*j*}:

$$\frac{\Delta P_j}{L} = \Phi u_j \quad (5)$$

$$\text{HETP}_j = A + B u_j + C / u_j$$

where $u_j = Q_j / \Omega$ is the superficial velocity in the j -th section and A , B , C and Φ are constants depending only on physical properties.

As a first step of the optimisation procedure, the following three statements are made:

1. The cross section of the columns, Ω , is the scale parameter of the plant. It is assumed equal to 1 m² to perform the calculations using flow-rates in m³/s equivalent to velocities in m/s. The actual value of Ω is calculated in order to reach the desired feed flow-rate: $\Omega = Q_F / Q_F$ ($\Omega = 1$). The remaining design parameters, m_j and L , are unchanged.

2. Since pressure drop is proportional to the throughput of the plant, we expect that productivity will be the highest when pressure drop is the highest possible in the plant. Therefore we set pressure drop in section 1, which is where the fluid velocity is maximum, equal to the allowable upper limit, hence fixing the value of the product u_1L and, together with Ω , the flow-rate in section 1.

3. From the adsorption isotherms it is possible to predict a priori the values of m_1 and m_4 which guarantee the proper behaviour of sections 1 and 4, i.e., complete regeneration of the eluent and the adsorbent, respectively, in the most general case of non linear adsorption isotherms. Note that in order to account for possible model inaccuracies, proper safety margins can be included [15].

Having chosen m_1 , m_4 and Q_1 and using Ω as scale parameter, only three of the seven original degrees of freedom of the SMB remain to be fixed: the column length and the flow-rate ratios m_2 and m_3 . For this, we develop an optimisation algorithm with productivity as objective function and with extract and raffinate purities as constraints.

The algorithm is based on the physically intuitive argument that purity values *higher* than those required would lead to a productivity value lower than that reachable with purity *equal* to the required ones. As a reference for the operating conditions the predictions of equilibrium theory were used. The optimum operating point predicted by equilibrium theory corresponds to the point of the complete separation region drawn in the (m_2, m_3) plane which lies further from the diagonal [16–18].

In this frame we define the new parameter η as the ratio between the actual feed flow-rate, made non-dimensional with respect to the flow-rate in section 1, and the optimal one predicted by equilibrium theory:

$$\eta = \frac{m_3 - m_2}{m_{3,\text{Eq.Th.}} - m_{2,\text{Eq.Th.}}} \quad (6)$$

In practice η corresponds to the dimensionless distance from the diagonal in the (m_2, m_3) plane of the chosen operating point, being $\eta=1$ the distance of the vertex of the complete separation region predicted by equilibrium theory.

The adopted strategy is to first fix a value for η .

With this, we proceed to compute the values of L and m_2 (and therefore all the other SMB characteristics with the appropriate equations), that lead to the required, and not higher, purity values. With this we construct a plot of productivity versus η and get the final optimal operation point as the value of η which maximises productivity.

The algorithm, which is shown in Fig. 2, involves two convergence loops, an inner one on m_2 and an outer one on L . This also allows accounting in each section for different values of HETP and number of theoretical plates, which instead are assumed often constant in similar types of calculations [13,14].

Let us now describe in detail the development of the proposed algorithm.

For each value of η , a sufficiently low initial value for the column length is chosen. With this column length, m_2 is changed until both purities are either inside or outside the required limits (inner loop), as depicted in Fig. 3 on the left-hand side. If both purities are not satisfactory, the efficiency is not enough and the column length should be increased (outer loop), in order to increase the size of the region where the purity satisfies the requirements (cf. Fig. 3, right-hand side). On the other hand, if the purities are above the purity requirements the column length is too large and the productivity cannot be at its maximum, so we increase L stepwise in order to enter this area staying close to the boundary. The procedure is repeated until the outlet stream purities are the expected ones.

Thus summarising, the developed procedure starts with a low L value and searches in m_2 if a condition that satisfies both purity requirements exists. If this does not exist, L is increased until the value where such a condition is found. Since this is for the smallest value of L , it guarantees that we have the maximum productivity for the selected value of η .

3.1. Description of an illustrative optimisation calculation

Let us consider for example $\eta=0.7$ and a purity requirement equal to 99% for both outlet streams of a unit whose properties are summarised in Table 1. In Fig. 4 we show, as a function of m_2 , the purities in extract and in raffinate obtained for two different values of L . It is seen that for $L=18.6$ cm, no value

$m_{2,opt}$ and $m_{3,opt}$ are known from equilibrium theory.
 $\eta = (F/Q_1) / (F/Q_1)_{opt}$
 m_1 and m_4 are fixed from the thermodynamic properties.
 Ω is the scale parameter of the plant and is assumed equal to 1.
 ΔP_{max} is given.

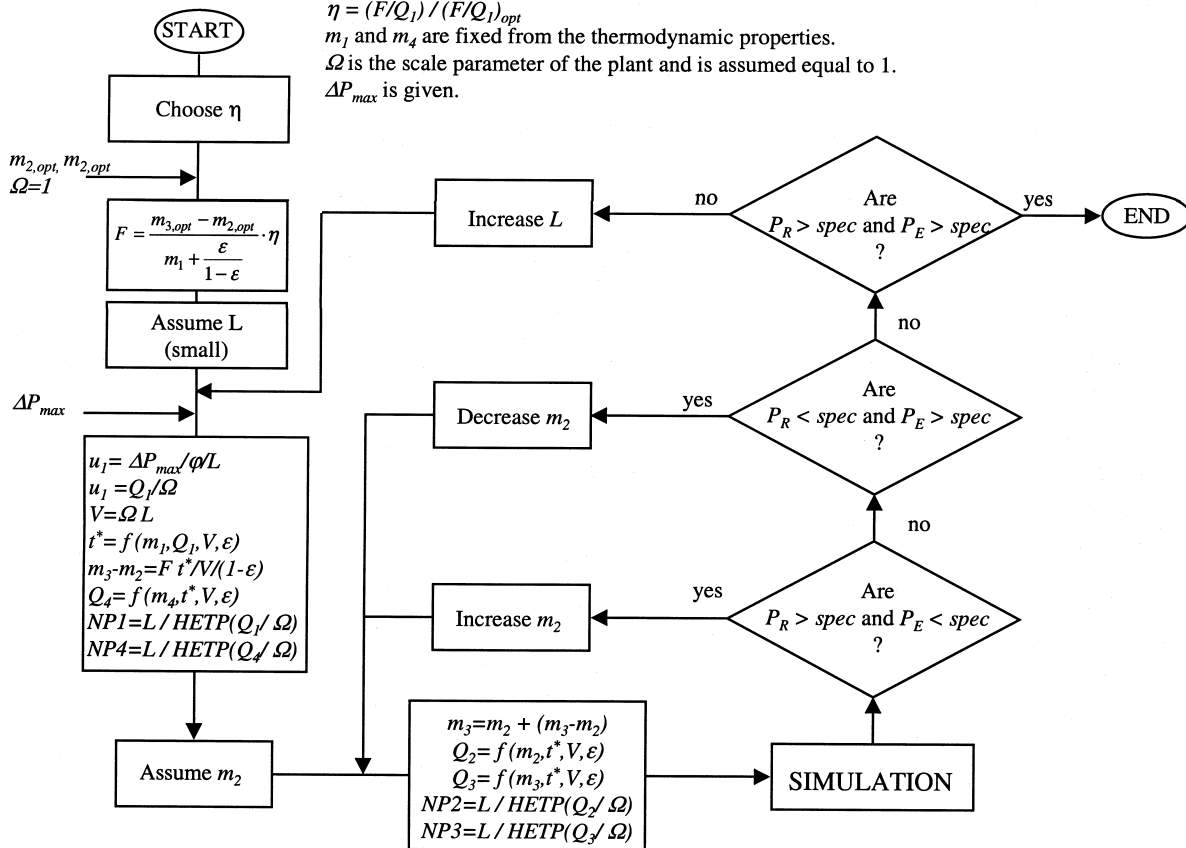


Fig. 2. Diagram of the optimisation algorithm.

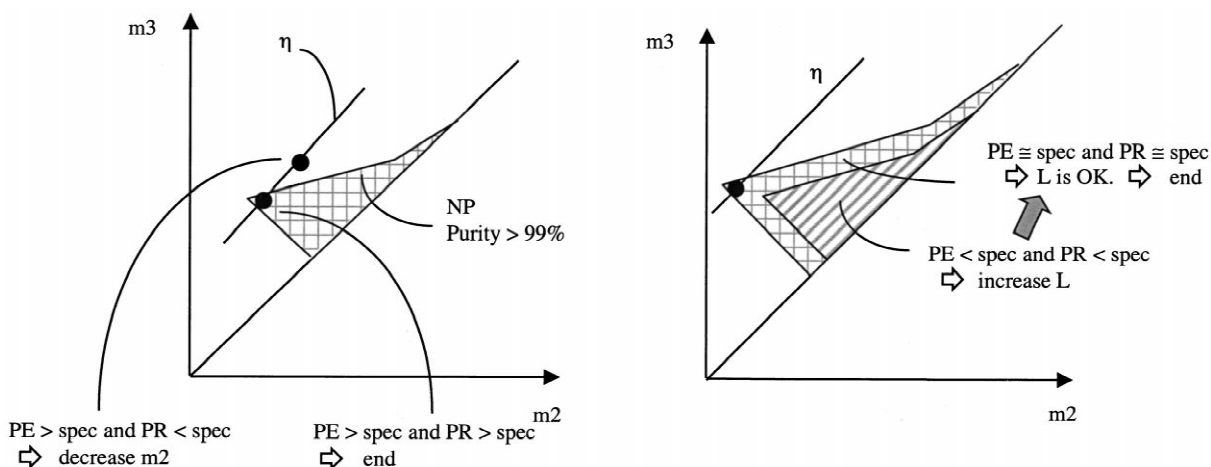


Fig. 3. Effect of the column length L and of η on the purities, represented with the aid of the operating plane (m_2, m_3) .

Table 1
Summary of the properties of the system, to which the optimisation procedure has been applied

External porosity:	$\epsilon_b = 0.565$
Internal porosity:	$\epsilon_p = 0$
Isotherms:	$q_1 = \frac{1.25 \cdot c_1}{1 + 0.125 \cdot c_1 + 0.1c_2}$ $q_2 = \frac{1 \cdot c_2}{1 + 0.125 \cdot c_1 + 0.1c_2}$
Configuration of columns:	2–2–2–2
Maximum allowed pressure drop:	$\Delta P_{\max} = 60$ bar
Van Deemter equation:	HETP (cm) = $0.01 + 0.678u$ (cm/s)
Pressure drop correlation:	ΔP (bar) = $2.4u$ (cm/s) · L (cm)

of m_2 provides purities P_E and P_R which are both larger than the required ones, i.e., 99%. Therefore we have to increase L . In fact for the value $L = 18.7$ cm we found an m_2 value, which is about 0.952. The column length L that leads to purity values both

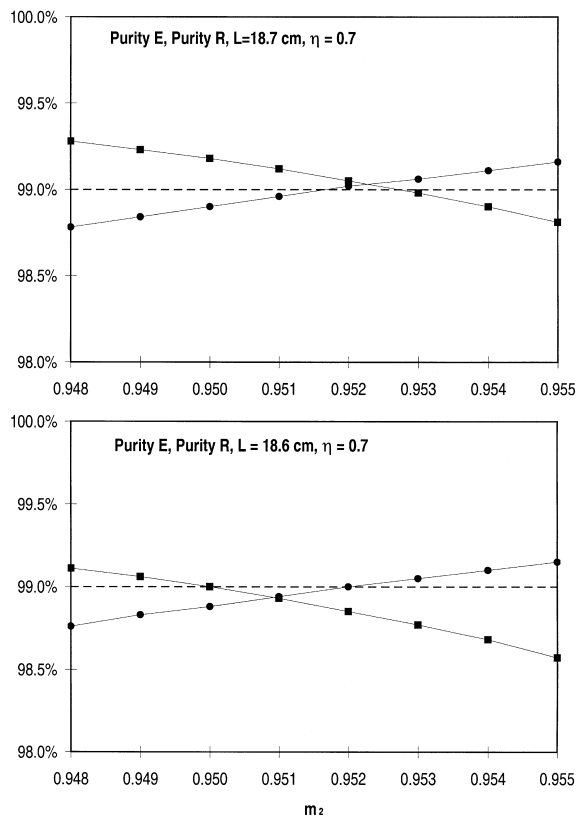


Fig. 4. Choice of column length for a given η : effect of m_2 on purity of the outlet streams.

equal to the specifications with $\eta = 0.7$ is then between 18.6 and 18.7 cm.

The computations above are repeated for various values of η leading to the plot shown in Fig. 5, from which the optimal operating condition is readily obtained for $\eta = 0.9$, as the one maximising productivity. In the same figure the required column length is also represented: typically L only slowly changes as long as the value of η is quite lower than the optimal one. In this range productivity increases almost linearly. When the optimal value of η is approached, the needed column length increases and the slope of the function productivity vs. η decreases until the maximum is reached, for $\eta = 0.9$ and $L = 20.4$ cm. These are the optimal design parameters and therefore they are the result of this design procedure, with purity requirement equal to 99%. The optimal column section is then obtained by scaling the flow-rates and the column volume in order to reach the specified production rate ($c_{T,F}Q_F$), while keeping column length and velocities in all sections constant.

4. Results and discussion

4.1. Effect of purity requirements

The proposed design method has been applied to analyse how the optimal design parameters are influenced by the specified purity requirements. It is shown in Fig. 6 how the maximum productivity changes by varying the required purity, which has been imposed to be the same for both, raffinate and extract streams: it is indeed not surprising that productivity decreases as the required purity increases. The calculations have been performed for a system with selectivity equal to 1.25, whose properties are reported in Table 1. The feed concentration was 10 g/l for the two compounds present in the mixture; the molecular diffusion term c in the Van Deemter equation was neglected, as it can be usually done for the velocities and particle sizes usually adopted in HPLC. It can be seen that with these data the productivity becomes about 10-times larger when we reduce the purity specifications from 99 to 80%.

Since the separation performance is more critical when high purity is required, the number of theoret-

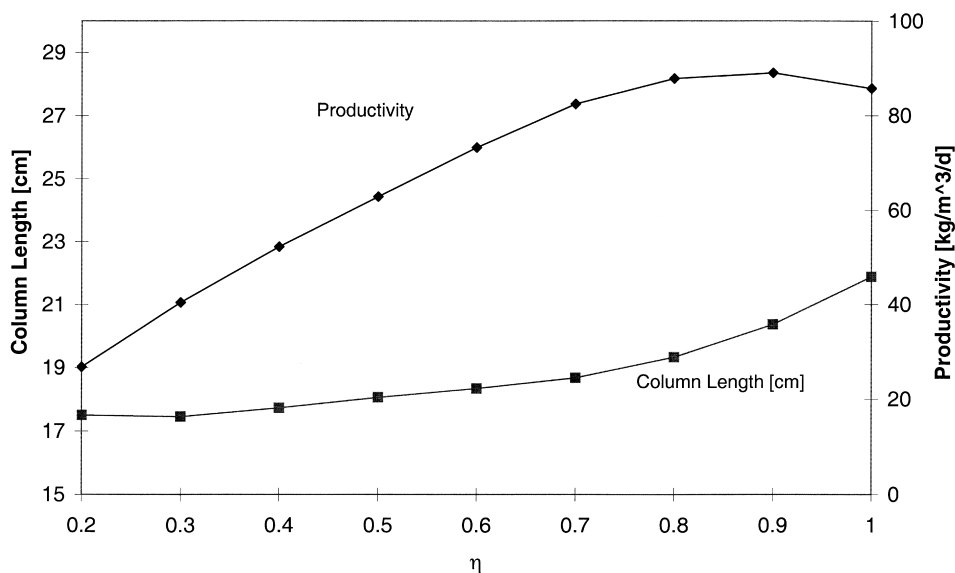


Fig. 5. Productivity and optimal column length as functions of η with purity equal to 99% for the system described in Table 1. The maximum corresponds to the optimal operating point.

ical plates and therefore the column length increase when the required purity increases, as shown in Fig. 7. On the other hand the optimal value of η increases when purity decreases, as seen in Fig. 8. The corresponding points in the operating plane (m_2, m_3)

are represented in Fig. 9. They are all lined up on a single line, which goes through the vertex of the complete separation region predicted by the equilibrium theory. For 99% purity in both outlet streams, the optimisation leads to $\eta=0.9$ and the optimal

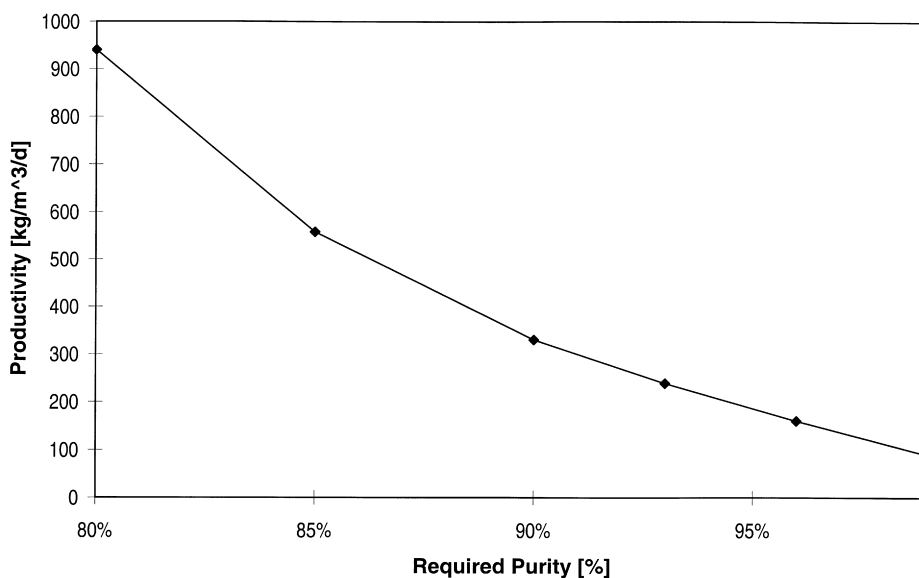


Fig. 6. Maximal productivity for various purity specifications for the system described in Table 1.

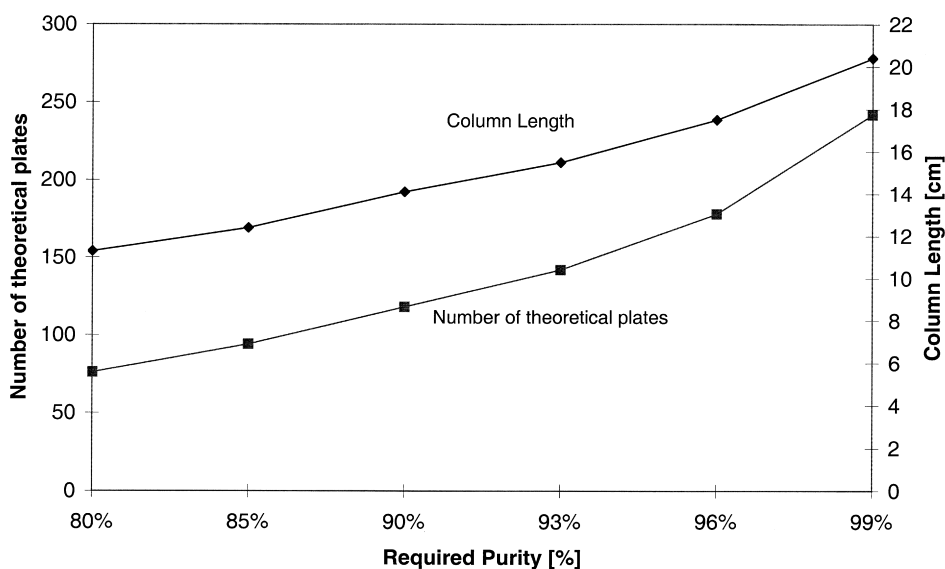


Fig. 7. Optimal column length and number of theoretical plates with various purity specifications for the system described in Table 1.

operating point in the (m_2, m_3) plane is inside the complete separation region according to equilibrium theory. With a purity requirement of about 98%, $\eta=1$ and the optimal operating point coincides with the prediction of equilibrium theory. Thus, somehow the purity decrease with respect to the complete

separation (i.e., 100% purity) predicted by the equilibrium theory compensates for the effects of dissipation terms. For lower purity requirements the optimal η is greater than one and therefore the optimal operating points are all outside the complete separation region, in the region where neither pure

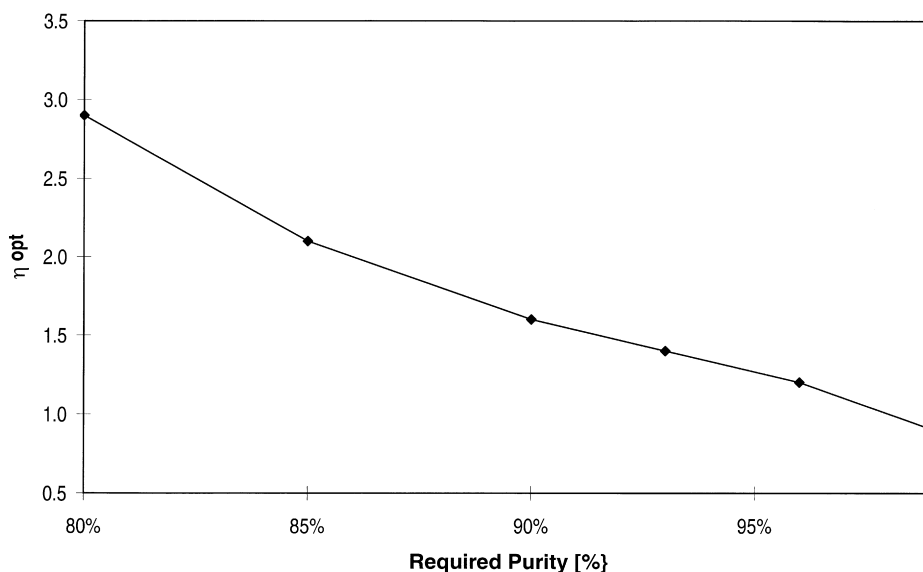


Fig. 8. Values of η leading to the maximal productivity for various purity specifications for the system described in Table 1.

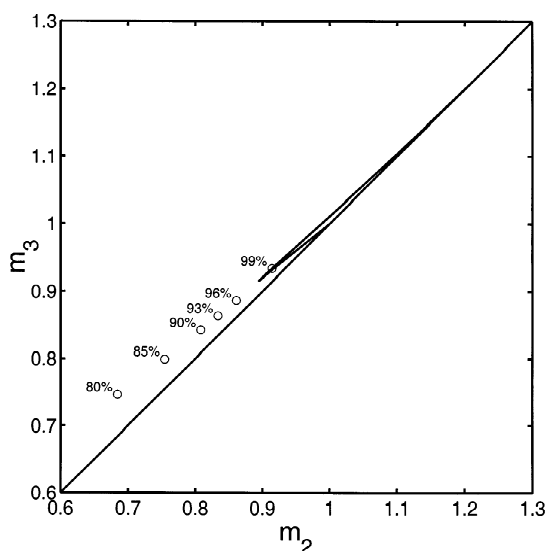


Fig. 9. Optimal operating points in the plane (m_2 , m_3) for various purity specifications compared with the complete separation region predicted by equilibrium theory.

extract nor pure raffinate is predicted by equilibrium theory.

4.2. Effect of particle size

Changing particle size is assumed to influence only the coefficients in the pressure drop correlation and in the Van Deemter equation (Eq. (5)). The permeability of the column $1/\Phi$ is assumed to be proportional to the square of particle diameter, according to the Blake–Kozeny equation, which holds true for laminar flow regime [19]:

$$\frac{\Delta P}{L} = \frac{(1 - \epsilon_b)^2}{\epsilon_b^3} \cdot \frac{150\mu}{d_p^2} u = \frac{\varphi}{d_p^2} \cdot u = \Phi u \quad (7)$$

where u is the superficial fluid velocity, μ the fluid viscosity and d_p the particle diameter.

Under ordinary HPLC operating conditions the molecular diffusion term in Van Deemter's equation can be neglected (i.e., $C=0$ in Eq. (5)), while it is assumed that the Eddy diffusion term A is proportional to particle size. About the effect of interparticle mass transfer resistances, since the fluid velocity is usually very small, the following value for the Sherwood number can be used:

$$\text{Sh} = \frac{d_p k_e}{D_m} = 2 \quad (8)$$

where k_e is the external mass transfer coefficient, D_m is molecular diffusivity. This must be combined with the intraparticle mass transfer resistance, which, using Glueckauf relation, leads to the following expression of the characteristic time of mass transfer:

$$\tau = \frac{d_p}{6k_e} + \frac{d_p^2}{60D_p} = \left(\frac{1}{12D_m} + \frac{1}{60D_p} \right) \cdot d_p^2 \quad (9)$$

where D_p is the pore diffusivity [20].

Since it is found that both resistances imply a second order dependence on the particle diameter, the following expression for the Van Deemter equation can be used:

$$\text{HETP} = A + Bu = ad_p + bd_p^2 u \quad (10)$$

where the dependence on the particle diameter has now been made explicit.

Several optimisation calculations have been performed by changing the particle diameter according to Table 2. The adsorption isotherms and the plant configuration were the same as in the previous calculations (cf. Table 1). In Figs. 10 and 11 it is observed that for various purity requirements the optimal column length increases and the corresponding productivity decreases when particle size increases. In all cases, the required number of plates and the corresponding optimal values of m_2 , m_3 and therefore η calculated for the same purity requirements are the same, as is shown in Table 3 for purity equal to 99%.

Moreover, it can be shown that as long as the molecular axial diffusion does not play an important role in determining the efficiency of the column, the productivity keeps increasing when particle diameter is reduced. However, when the molecular diffusion

Table 2

Summary of the pressure drop correlation coefficient and of the Van Deemter parameters estimated for different particle diameters

Particle diameter (μm)	Φ	A	B
20	2.4	0.01	0.678
40	0.6	0.02	2.712
80	0.15	0.04	10.85
160	0.038	0.08	43.39

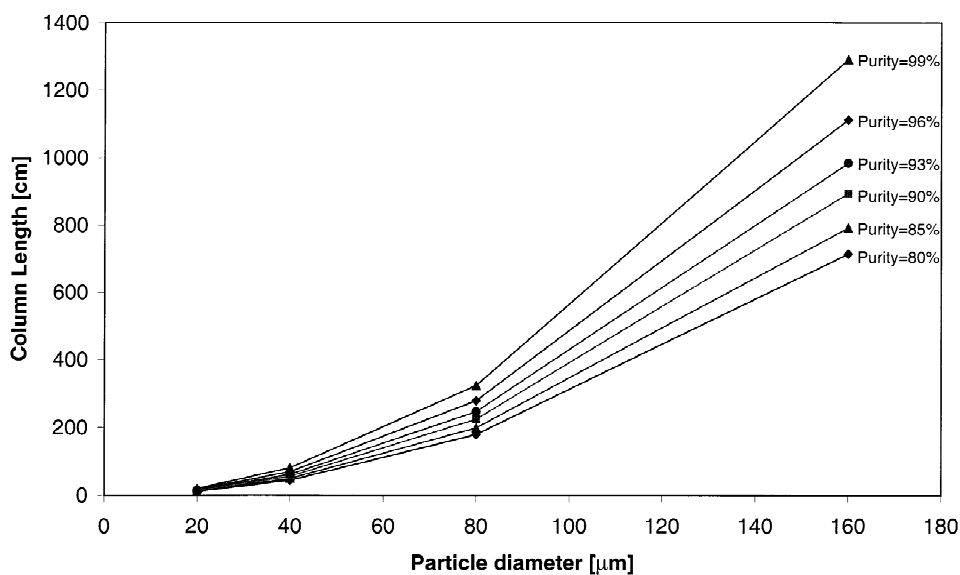


Fig. 10. Optimal column length as a function of particle size for various purity specifications for the system described in Table 1.

term is important it is possible to show the existence of a maximum in the productivity vs. particle diameter plot. This can be intuitively understood, if we consider that having a small particle diameter implies having a relevant pressure drop already with short columns. Therefore, in order to comply with

the pressure drop constraint one must operate with very low velocities, in a condition where molecular diffusion is not negligible. The resulting behaviour is depicted in Fig. 12, where the results of several calculations are shown for a system having the properties reported in Table 1 but having the follow-

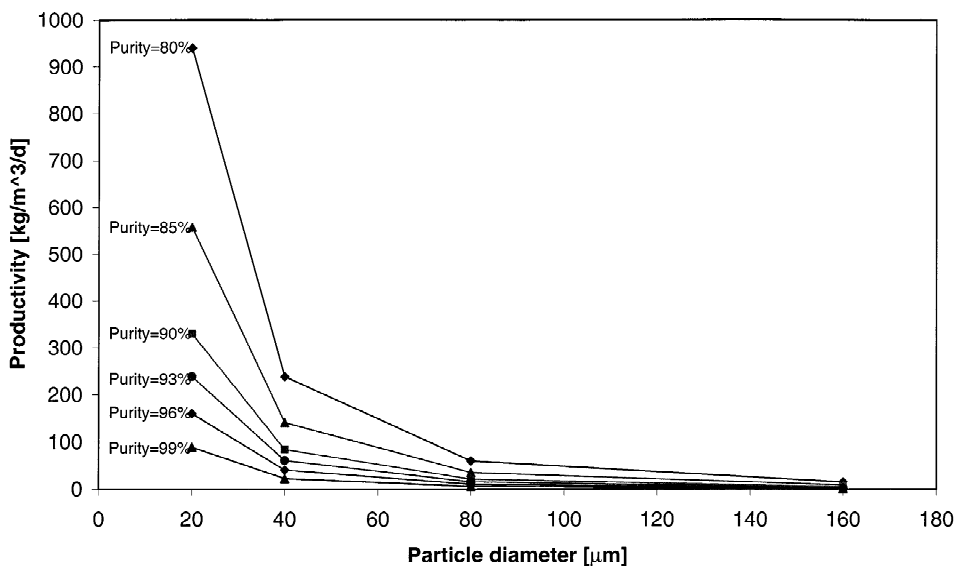


Fig. 11. Maximal productivity as a function of particle size for various purity specifications for the system described in Table 1.

Table 3
Summary of the results of the optimisation for different particle diameters

Particle diameter (μm)	m_2	m_3	NST_1	NST_2	NST_3	NST_4	Productivity ($\text{kg}/\text{m}^3/\text{d}$)	L (cm)
20	0.914	0.933	24	30	30	37	89	20.4
40	0.914	0.933	23	30	30	37	23	80.9
80	0.914	0.933	23	30	30	37	6	323
160	0.914	0.933	23	30	30	37	1.4	1290

ing Van Deemter equation and pressure drop dependence:

$$\text{HETP} = 0.0005d_p + 0.00165d_p^2u + 0.001/u$$

$$\frac{\Delta P}{L} = \frac{960}{d_p^2} \cdot u \quad (11)$$

(HETP and L are in cm, d_p is in μm , u is in cm/s).

It is seen that there is a maximum of productivity corresponding to a particle size around $3 \mu\text{m}$. This is strictly related to the fact that the effect of molecular diffusion starts being comparable to the other contributions to HETP.

What is more, when u approaches 0, Eqs. (5) and (7) yield $\text{HETP} \approx C/u$ and:

$$\lim_{L \rightarrow +\infty} NP = \frac{\Delta P_{\max}}{\Phi C} = \frac{\Delta P_{\max}}{\varphi C} \cdot d_p^2 \quad (12)$$

Under these conditions molecular diffusion is dominant, therefore increasing the column length in order to increase efficiency is useless, because the fluid velocity must also be reduced to avoid exceeding the pressure drop limit and therefore the HETP also increases leading to the same number of plates. Thus, there exists an upper limit in the number of stages that can be obtained for each value of d_p . This limit decreases with d_p : therefore below a certain particle size, the number of plates needed to achieve the desired purity cannot be reached anymore whatever the column length and the operating conditions. With the data we used, this happens for a particle diameter between 1 and $2 \mu\text{m}$, as illustrated in Fig. 12.

This behaviour is general, even if with the data used for the calculations this could be observed only with unrealistic values for column length and switch

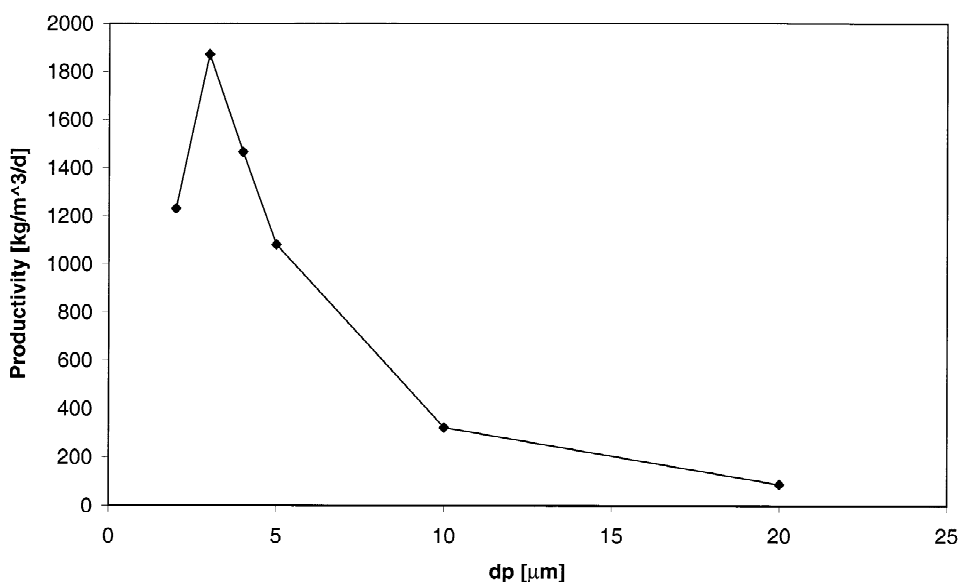


Fig. 12. Maximal productivity as a function of particle size in a system where axial diffusion is relevant.

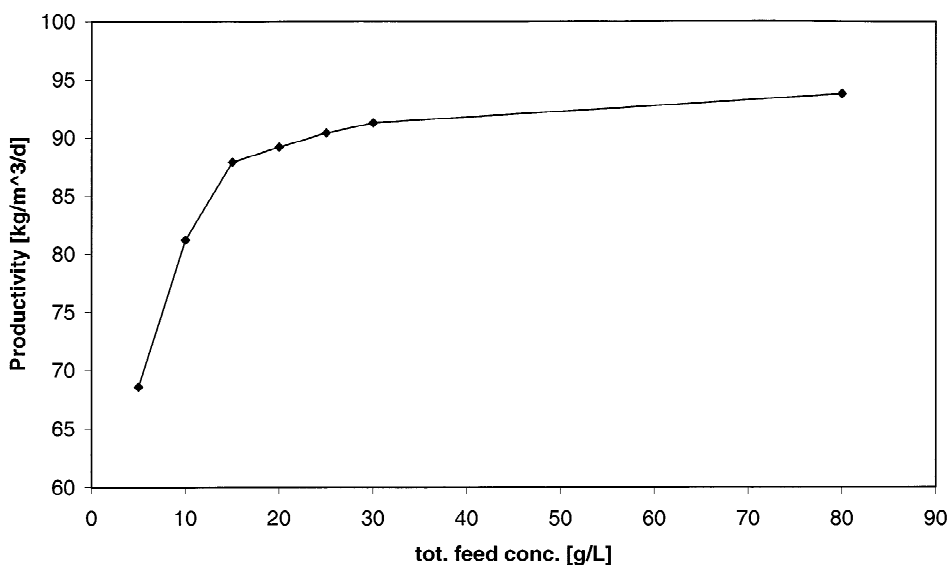


Fig. 13. Maximal productivity calculated for different feed concentrations.

time. In practice too short columns cannot be packed properly and too short switch times do not allow the system to stabilise between two switches and the minimal values of L and t^* that can be realised condition the choice of the particle size. For this reason we do not consider it convenient to regard the particle size as a free optimisation parameter and we decided to analyse its influence on the separation separately.

4.3. Effect of feed concentration

The developed procedure has been used also to investigate the effect of feed concentration on productivity. Similarly to what can be theoretically predicted with equilibrium theory and to the conclusions driven by Charton and Nicoud [13], one observes an asymptotic behaviour: productivity keeps increasing when feed concentration is increased, but the increase becomes smaller and smaller, as is represented in Fig. 13 for the system whose properties are summarised in Table 1. This behaviour implies that the highest possible feed concentration compatible with solubility limitations is the optimal one.

However, these predictions could be used directly only if all the parameters were known in a de-

terministic way, which is obviously not true. From equilibrium theory we expect the robustness of the working conditions to become lower when feed concentration is increased [14]. Therefore, the choice of the actual feed concentration cannot be made without considering all possible sources of disturbance and uncertainty: therefore only if the feed concentration is low enough, the predictions of the model can be implemented in practice.

What is more, in several cases the solubility of the mixture is the limiting constraint for feed concentration. The most important suggestion for selecting $c_{F,T}$, then, is that the conditions of choice must be far away from precipitation. In general, therefore, it can be concluded, that criteria different from maximal productivity, whose definition is beyond the scope of this work, are used for choosing feed concentration.

5. Conclusions

In this work we developed a logic procedure to design both a SMB unit and its operating conditions, with an overall view on equilibrium properties, kinetics and fluid dynamics. This allows us to determine the highest productivity that can be reached for a given separation with given constraints

on purity and on pressure drop and accounting for the real efficiency of the unit. Combining optimisation of the size of the unit and of the operating conditions of the separation represents a significant improvement with respect to previous analysis of the non ideal effects on SMB performance [13,21–26].

Calculations have been performed in different conditions and the results have been compared with the predictions of equilibrium theory. This has shown that in general the optimum set of parameters according to the new procedure does not coincide with the predictions of equilibrium theory: the optimum value of η is not 1 and depends on the actual values of parameters that are not considered in equilibrium theory.

In particular, the new algorithm has been used to study the effect on the separation performance of some of these parameters, such as particle diameter and purity requirement. It has been shown how strong the influence of purity requirements on working conditions and productivity is. The effect of particle size and the role of the feed concentration have been also investigated considering their influence on the operating conditions and on the separation performance. The reason why these were not included as optimisation variables in the design procedure has been discussed.

In this way we have shown that a versatile optimal design tool for non linear SMBs is made available not only for a given plant but also for new separations.

References

- [1] D.B. Broughton, US Pat. 2 985 589 (1961).
- [2] D.M. Ruthven, C.B. Ching, *Chem. Eng. Sci.* 44 (1989) 1011.
- [3] R.M. Nicoud, *LC·GC Int.* 5 (1992) 43.
- [4] R.M. Nicoud, *Pharm. Tech. Europe* 2 (3) (1999) 36.
- [5] R.M. Nicoud, *Pharm. Tech. Europe* 2 (4) (1999) 29.
- [6] E. Francotte, P. Richert, *J. Chromatogr. A* 769 (1997) 101.
- [7] E. Cavoy, M.F. Deltent, S. Lehoucq, D. Miggiano, *J. Chromatogr. A* 769 (1997) 49.
- [8] M.P. Pedferri, G. Zenoni, M. Mazzotti, M. Morbidelli, *Chem. Eng. Sci.* 54 (1999) 3735.
- [9] R.M. Nicoud, in: G. Subramanian (Ed.), *Bioseparation and Bioprocessing*, Vol. 1, Wiley-VCH, 1998.
- [10] M. Mazzotti, R. Baciocchi, G. Storti, M. Morbidelli, *Ind. Eng. Chem. Res.* 35 (1996) 2313.
- [11] M. Juza, O. Di Giovanni, G. Biressi, V. Schurig, M. Mazzotti, M. Morbidelli, *J. Chromatogr. A* 813 (1998) 333.
- [12] J.Y. Clavier, R.M. Nicoud, M. Perrut, *High Pressure Chemical Engineering*, Elsevier, London, 1996.
- [13] F. Charton, R.M. Nicoud, *J. Chromatogr. A* 702 (1995) 97.
- [14] O. Ludemann-Hombourger, M. Bailly, R.M. Nicoud, *Sep. Sci. Technol.*, (2000) in press.
- [15] C. Migliorini, M. Mazzotti, M. Morbidelli, *J. Chromatogr. A* 827 (1998) 161.
- [16] M. Mazzotti, G. Storti, M. Morbidelli, *AIChE J.* 40 (1994) 1825.
- [17] M. Mazzotti, G. Storti, M. Morbidelli, *AIChE J.* 42 (1996) 2784.
- [18] M. Mazzotti, G. Storti, M. Morbidelli, *J. Chromatogr. A* 769 (1997) 3.
- [19] R.B. Bird, W.E. Stewart, E.N. Lightfoot, in: *Transport Phenomena*, Wiley, 1960, p. 199.
- [20] M.D. LeVan, G. Carta, C.M. Yon, in: R.H. Perry, D.W. Green, J.O. Maloney (Eds.), *7th Edition, Perry's Chemical Engineer's Handbook*, Vol. 1, McGraw-Hill, 1997, pp. 42–43.
- [21] Z. Ma, N.-H.L. Wang, *AIChE J.* 43 (1997) 2488.
- [22] G. Zhong, G. Guiochon, *Chem. Eng. Sci.* 52 (1997) 3117.
- [23] L.S. Pais, J.M. Loureiro, A.E. Rodrigues, *J. Chromatogr. A* 827 (2) (1998) 215.
- [24] C. Migliorini, A. Gentilini, M. Mazzotti, M. Morbidelli, *Ind. Eng. Chem. Res.* 38 (1999) 2400.
- [25] D.C.S. Azevedo, A.E. Rodrigues, *Ind. Eng. Chem. Res.* 38 (1999) 3519.
- [26] D.C.S. Azevedo, A.E. Rodrigues, *AIChE J.* 45 (5) (1999) 956.