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HYBRID DYNAMIC OPTIMISATION: CASE STUDY OF A PRESSURE SWING ADSORPTION PROCESS

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Abstract: In this paper, a hybrid dynamic optimisation approach is developed for simulation of a pressure swing adsorption (PSA) process. The simulation problem which consists in the determination of the cyclic steady-state (CSS) is formulated as an optimisation problem where the performance index is the CSS condition, the decision variables are the state variables at the start of the cycle and the process model along with associated initial and boundary conditions gives the constraints. The necessary conditions of optimality for the hybrid dynamic system using the adjoint system method are derived and the gradients are computed for the non linear programming (NLP) solver used. The optimisation results are compared to those obtained with gradients computed by means of finite differences method.

Keywords: Dynamic optimisation, hybrid system, PSA, Adjoint system method

1. INTRODUCTION

The class of hybrid processes considered in this paper refers to processes that require the use of different process models, each is valid in a given functioning time domain. Transitions between domains take place at different time instants (events). Examples of hybrid processes include pressure swing adsorption processes, reverse flow reactors, small-size waste water treatment plants, etc.

In general, this class of hybrid processes is described by time-dependent, non-linear dynamic models that exhibit model switching as a sequence of both time and state-dependent events.

A pressure swing adsorption process consists of four basic operations (typical Skarstrom cycle), i.e. pressurisation, high pressure adsorption, blow down and low pressure purge. This sequence of operations is carried out in a series of fixed-beds in the same way but shifted in time. PSA processes are therefore transient and cyclic in nature.

The PSA process models are described by sets of partial differential algebraic equations (PDAEs). They are mainly constituted by conservation equations and models for the equation of state, equilibrium and thermodynamic and transport properties.

The simulation of PSA processes consists in the determination of the cyclic steady-state. This is traditionally performed by means of successive substitution or Newton-type methods. These methods are well known in the literature and are extensively studied in order to improve their robustness and convergence rate. However, alternative and interesting approaches have recently emerged and are based on the use of optimisation methods for the determination of CSS (Nilchan and Pantelides (1998), Jiang et al. (2003), Ko et al. (2003), Ko et al. (2005), Latifi et al. (2008)).

Their basic principle consists in the formulation of the simulation problem as a dynamic optimisation problem where the performance index is defined as the sum of square differences between the state variables (gas phase concentrations, solid-phase concentrations and temperature) obtained at the beginning and at the end of a cycle. The decision variables are the initial conditions (state variables at the beginning of a cycle), and the constraints are given by the process model where the method of lines is used for spatial discretisation and converts the PDAEs to differential-algebraic equations (DAEs). A gradient-based nonlinear programming (NLP) solver is then used to determine the initial state vector which minimises the cyclic steady-state condition.

The main differences between the previous works on optimisation-based simulation of PSA processes are the method of discretisation of PDAEs (both single discretisation and complete discretisation) and the method used to compute the gradients for the NLP solver.

In (Nilchan and Pantelides (1998), Ko et al. (2003)) the complete discretisation approach, i.e. space and time are discretised, is used and the resulting NLP problem is solved within the sensitivity-based code gPROMS. For simple models this approach is efficient, but for complicated models the complete discretisation causes error accumulation and may lead to solver failure.

In (Ko et al. (2003), Ko et al. (2005), Jiang et al. (2003)) the single discretisation approach where only the space is discretised is used and the method of lines used is the centred finite differences in (Ko et al. (2003), Ko et al. (2005)) whereas the finite volume method is used in (Jiang et al. (2003)). In the three works, the sensitivity method is used and the resulting optimisation problem is solved within gPROMS. It is important to notice that the spatial discretisation method involves a quite large number of decision variables and the use of sensitivity method for gradients computation results in a huge DAE system and consequently in big computation times. On the other hand since the number of constraints involved in an optimisation-based determination of CSS is small , the adjoint system method becomes more interesting.

In (Latifi et al. (2008)) the spatial discretisation approach used is based on orthogonal collocation method and the adjoint system method is used for gradients computation. They showed that the adjoint method has the fastest convergence rate compared to finite differences method and both numerical and analytical sensitivity methods. However, orthogonal collocation methods often introduce physically unrealistic oscillations near steep adsorption fronts and lead to solutions with negative values for positive variables (e.g. mole fractions). The finite volume method allows us to determine accurate solutions which in addition preserve the mass and energy balance in the spatial direction (conservative method).

The objective of this paper is the simulation of PSA processes, i.e. determination of the cyclic steady-state, by means of a hybrid dynamic optimisation approach which relies on high-quality system models. Moreover, the objective is : (i) to derive the necessary conditions of optimality for a hybrid system using the adjoint method and to deduce the gradients required by the NLP solver, (ii) to formulate the simulation of PSA processes as a hybrid dynamic optimisation problem where the model PDAEs are converted to DAEs using the finite volume method (iii) and to present some new results obtained in the case of a non isothermal PSA process.

2. MATHEMATICAL REPRESENTATION OF HYBRID SYSTEMS

The formalism used here to model the hybrid systems under consideration is derived from (Galàn et al. (1999) and Ruban (1997)). We consider a system described by a state space $S = U_{k=1}^{n_k} S_k$, where each mode S_k is characterised by :

(1) A set of variables $\{\dot{x}^{(k)}, x^{(k)}, p\}$, where $x^{(k)}(p,t)$ are the differential state variables, p the time-independent parameters, and t the time that varies in $[t_o^{(k)}, t_f^{(k)}]$.
(2) A set of equations $f^{(k)}(\dot{x}^{(k)}, x^{(k)}, p) = 0$, usually coupled system of differential and algebraic equations.
(3) A set of transitions to other modes. These transitions are described by :
   - Transition conditions $L_j^{(k)}(\dot{x}^{(k)}, x^{(k)}, t_f^{(k)}, p) = 0$, $j = 1, 2, ..., n_s$, determining the transition times at which switching from mode k to mode j occurs. The transition conditions are represented by logical propositions that trigger the switching when they become true.
   - Associated with these transition conditions are sets of transition functions $x^{(k+1)} = x^{(k)} + \Delta_j^{(k)}(x^{(k)}, t_f^{(k)}, p)$ relating the variables in the mode S_k and the variables in the new mode S_j at transition time $t_f^{(k)}$. A special case of the transition functions is the set of initial conditions for the initial mode S_1.

3. PSA PROCESS MODEL

The hybrid system considered here is a PSA process for air drying by silica gel. The process used consists of four steps : instant pressurisation, high pressure adsorption,instant blow down and low pressure purge. The process model is similar to that in (Chihara and Suzuki (1983)) and is based on the following assumptions:

- A monodimensional model is considered.
- The system is non isothermal.
- The axial dispersion is negligible.
- The gas phase is ideal.
- The carrier gas is assumed to be inert.
- The mass transfer rate is described by LDF (linear driving force) model.
- Frictional pressure drop is negligible.
- Fluid phase and solid phase are in thermal equilibrium.
- The effect of temperature change on gas and solid properties is negligible.

The resulting model is constituted by the following equations:

1. Adsorbate mass balance in the fluid phase :

$$v\frac{\partial c}{\partial z}+\frac{\partial c}{\partial t}+\frac{\gamma}{\epsilon}\frac{\partial q}{\partial t}=0 \tag{1}$$

2. Mass transfer rate :

$$\frac{\partial q}{\partial t}=\frac{K_s a_v}{\gamma}(q^\star-q) \tag{2}$$

3. Adsorption equilibrium relationship :

$$q^\star=kc \tag{3}$$

The effect of temperature change on adsorption coefficient is described by :

$$\ln\frac{k}{k_o}=\frac{Q}{R}(\frac{1}{T}-\frac{1}{T_o}) \tag{4}$$

4. Energy balance :

$$\begin{aligned}\frac{k_{ez}}{\epsilon}\frac{\partial^2 T}{\partial z^2}-v\rho_g C_{pg}\frac{\partial T}{\partial z}+\frac{2h_o}{\epsilon r}(T_o-T)-\\ (\rho_g C_{pg}+\frac{\gamma}{\epsilon}C_{ps})\frac{\partial T}{\partial t}+\frac{\gamma}{\epsilon}Q\frac{\partial q}{\partial t}=0\end{aligned} \tag{5}$$

where $v=v_H$ for adsorption,

and $v=-v_L=-\alpha v_H$ for purge.

The associated boundary conditions for adsorption are:

$$c=c_o,\ T=T_o\ at\ z=0 \tag{6}$$

and for purge :

$$c=\frac{P_L}{P_H}c_{adsorption},\ T=T_o\ at\ z=L \tag{7}$$

Frozen solid state conditions are assumed during variable pressure steps, i.e pressurization and purge (Shendalman and Mitchell (1972)) for the PSA model under consideration. The pressure change during the steps of pressurization and blowdown is assumed so rapid that mass transfer between solid and fluid phases is negligible. Solid-phase concentration and temperature remain unchanged at the end of adsorption and purge steps whereas gas-phase concentration at the end of adsorption step is reduced in proportion to ratio of high pressure to low pressure. Gas-phase concentration remains unchanged at the end of purge step.

Equations (1 - 5) form a set of partial differential algebraic equations (PDAEs) which is converted in a set of partial differential equations (PDEs) since the system index is one (Unger et al. (1995), Brenan et al. (1996)).

4. SPATIAL DISCRETIZATION

The method of lines methodology (Schiesser (1991)) is used to convert the system of PDEs to a system of ordinary differential equations (ODEs). In this work, the finite volume method (Webley and He (2000)) is used. It is particularly suitable for modelling hyperbolic conservation laws given its inherent conservative properties (Leonard (1979)). The spatial domain is divided into a discrete number of volume elements and PDEs are integrated over volume element i

$$\int_{z_{i-1/2}}^{z_{i+1/2}} f(z)dz=\Delta_i\overline{f}_i \tag{8}$$

where Δ_i is the spatial length of volume element i and $\overline{f}_i$ is the control volume average of f in volume i. We assume that $\overline{f}_i=f_i$ where f_i is the value of f at the centre of control volume i. This scheme is illustrated in Figure (1) for a monodimensional model.

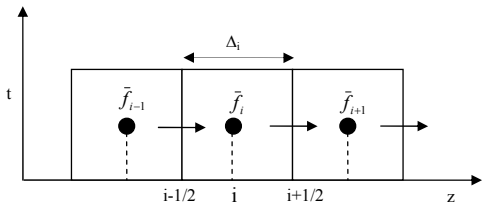

Figure 1. Monodimensional discretisation with finite volume method

The resulting process model may be written in the following ODEs :

$$\frac{d\bar{c}_i}{d\bar{t}}+\tau_a\frac{\bar{c}_{i+\frac{1}{2}}-\bar{c}_{i-\frac{1}{2}}}{\Delta\bar{z}}+\tau_b\frac{d\bar{q}_i}{d\bar{t}}=0 \tag{9}$$

$$\frac{d\bar{q}_i}{d\bar{t}}=\tau_f(\bar{q}^*-\bar{q}_i) \tag{10}$$

$$\bar{q}^{\star} = K\bar{c}_i \tag{11}$$

$$K = exp(-\frac{Q}{RT_o}(\frac{\bar{T}_i}{\bar{T}_i+1})) \tag{12}$$

$$\frac{d\bar{T}_i}{d\bar{t}} + \tau_H \frac{\bar{T}_{i+\frac{1}{2}} - \bar{T}_{i-\frac{1}{2}}}{\Delta\bar{z}} - \tau_L \frac{(\frac{\partial\bar{T}}{\partial\bar{z}})_{i+\frac{1}{2}} - (\frac{\partial\bar{T}}{\partial\bar{z}})_{i-\frac{1}{2}}}{\Delta\bar{z}} + \tau_W\bar{T}_i - \beta\frac{d\bar{q}_i}{d\bar{t}} = 0 \tag{13}$$

for $i = 1, 2, ..., N$

The boundary conditions in non-dimensional form are as follows:
For high-pressure adsorption :

$$\bar{c}_1 = 1,\ \bar{T}_1 = 0 \tag{14}$$

For low-pressure purge :

$$\bar{c}_N = \frac{P_L}{P_H}\bar{c}_{N(adsorption)},\ \bar{T}_N = 0 \tag{15}$$

The whole model of the PSA process under consideration illustrated in Figure (2) may be written in the following hybrid form :

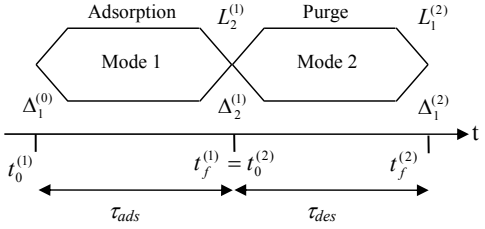

Figure 2. Schematic representation of the PSA process

$$\dot{x}^{(k)} = f^{(k)}(x^{(k)}, p) \tag{16}$$

The transitions conditions are :

$$L_j^{(k)} = t - t_f^{(k)} = 0 \tag{17}$$

The transitions functions associated with the transition conditions are :

- For fluid-phase concentration

$$x^{(k+1)}(t_o^{(k+1)}) = x^{(k)}(t_f^{(k)})\frac{P_L}{P_H} \tag{18}$$

- For solid-phase concentration and temperature

$$x^{(k+1)}(t_o^{(k+1)}) = x^{(k)}(t_f^{(k)}) \tag{19}$$

The special case of the transition functions is given by the initial conditions for the compression step (mode S_1) as

$$\Delta_1^{(0)} = x^{(1)}(t_0^{(1)}) - x_0^{(1)} = 0 \tag{20}$$

where the state vector is given by

$$x^{(k),T} = (\bar{c}_o^{(k)}, \bar{c}_1^{(k)}, .., \bar{c}_N^{(k)}, \bar{q}_o^{(k)}, \bar{q}_1^{(k)}, .., \bar{q}_N^{(k)}, \bar{T}_o^{(k)}, \bar{T}_1^{(k)}, .., \bar{T}_N^{(k)})$$

The initial state vector is given by

$$x_o^{(1),T} = (\bar{c}_o^{(1),o}, \bar{c}_1^{(1),o}, .., \bar{c}_N^{(1),o}, \bar{q}_o^{(1),o}, \bar{q}_1^{(1),o}, .., \bar{q}_N^{(1),o}, \bar{T}_o^{(1),o}, \bar{T}_1^{(1),o}, .., \bar{T}_N^{(1),o})$$

On the other hand, from the basic steps durations, i.e. τ_{ads} and τ_{des} , the transitions times are given as

$$t_f^{(1)} = \tau_{ads} \tag{21}$$

$$t_f^{(2)} = \tau_{ads} + \tau_{des} \tag{22}$$

The last transition time is also the PSA cycle duration.

5. OPTIMISATION-BASED FORMULATION OF THE SIMULATION PROBLEM

The objective of the simulation problem is to determine the cyclic steady-sate, i.e. the state vector at the start of the cycle must be equal to the state vector at the end of the cycle. The classical formulation of this objective is expressed as :

$$x^{(1)}(t_o^{(1)}) = x^{(2)}(t_f^{(2)}) \tag{23}$$

Different methods have been developed to solve (23), including fixed-point iteration approach, quasi-Newton and Newton methods (Smith IV and Westerberg (1991), Croft and LeVan (1994), Nilchan and Pantelides (1998)).

The optimisation-based formulation developed in this work consists in treating the simulation problem as a single dynamic optimisation problem where the performance index is the CSS condition, the decision variables are the state variables at the start of the cycle and the constraints are given by the hybrid model equations of the process with associated initial conditions.

It is noteworthy that the decision variables are the initial state vector. The time-independent vector of parameters is therefore defined as :

$$p = x^{(1)}(t_o^{(1)}) \tag{24}$$

The mathematical formulation of the optimisation-based simulation is given by :

$$\min_p \ J = \frac{1}{2} e^T e \tag{25}$$

$$where\ e = x^{(1)}(t_o^{(1)}) - x^{(2)}(t_f^{(2)})$$

Subject to constraints (16-20)

6. COMPUTATIONAL METHOD

The computational method used consists in estimating the initial values of decision variables which are used in process model integration. The performance index and the gradients of both performance index and constraints with respect to decision variables are computed and provided to a gradient-based NLP solver, which in turn estimates a new vector of decision variables. The process is repeated until convergence where the optimal values of decision variables are obtained.

It is important to notice that in any gradient-based optimisation solver, the convergence and its rate depend strongly on the accuracy of gradients computation. In this work, two methods are used and compared. They are based on the following general definition of the performance index:

$$\min_p \ J = G[x(t_f), p] + \int_0^{t_f} F[x(t), p] dt \tag{26}$$

6.1 *Finite differences method*

The approximation of the gradient of the performance index J with respect to a parameter p_i by means of (centered) finite differences method consists in perturbing J with a finite amount Δp_i of p_i as follows :

$$\frac{\partial J}{\partial p_i} = \frac{J(p_i + \Delta p_i) - J(p_i - \Delta p_i)}{2\Delta p_i} \tag{27}$$

where typically $\frac{\Delta p_i}{p_i} = 1\%$.

6.2 *Adjoint system method*

The gradient of the performance index J with respect to a parameter p_i by means of adjoint system method are derived from the results of (Bryson and Ho (1975) and Ruban (1997))

$$\frac{\partial J}{\partial p_i} = \lambda^1(t_o^{(1)}) \frac{\partial x^{(1)}(t_o^{(1)})}{\partial p_i} + \frac{\partial G}{\partial p_i} \tag{28}$$

The Hamiltonian function of the performance index in each mode is given by

$$H^{(k)} = F(x, p) + \lambda^T f^{(k)} \tag{29}$$

where the corresponding vector of adjoint variables is defined as

$$\dot{\lambda}^{(k)} = -\frac{\partial H^{(k)}}{\partial x^{(k)}} \tag{30}$$

with the terminal conditions

$$\lambda^{(2)}(t_f) = \left.\frac{\partial G}{\partial x}\right|_{t=t_f^{(2)}} = x^{(2)}(t_f^{(2)}) - p \tag{31}$$

The PSA process model under consideration is hybrid, consequently the corresponding adjoint system is also hybrid and the transition conditions and transition functions need to be taken into account for backward integration of the adjoint system.

The transition conditions (switching instants) for adjoint system are the same as for the process model. The corresponding transition functions are

- For fluid-phase concentration

$$x^{(k)}(t_o^{(k)}) = x^{(k+1)}(t_f^{(k+1)}) \frac{P_L}{P_H} \tag{32}$$

- For solid-phase concentration and temperature

$$x^{(k)}(t_o^{(k)}) = x^{(k+1)}(t_f^{(k+1)}) \tag{33}$$

The computational algorithm for adjoint system method is

(1) Estimation of initial values of decision variables p
(2) Integration of state equations (16-20)
(3) Backward integration of the system of adjoint equations (30-33)
(4) Computation of performance index by (26) and gradients by (28)
(5) Estimation of new vector of decision variables p by NLP solver and repetition of the process from step (2) until the convergence criteria is satisfied.

7. RESULTS

7.1 *Data used*

The durations of adsorption and purge steps are equal. The number of finite volume elements N is 20. The rest of physical data are given in Table (1) (Chihara and Suzuki (1983)).

7.2 *Results and discussion*

The simulations are carried out on a 3.40 GHz Intel Pentium 4 computer. The NLP solver used

Parameter	Value	Unit
L	1	m
r	0.1	m
ϵ	0.4	-
γ	7.2x10^3	kg/m^3
ρ_s	1.2x10^3	kg/m^3
C_{ps}	1.26x10^3	$J/kg.K$
ρ_g	1.2	kg/m^3 (at atm. pres.)
C_{pg}	1x10^3	$J/kg.K$
k	7.57	m^3/kg
Q	5.19x10^4	J/mol
$K_s a_v$	0.2	$kg/m^3.s(at\ P_H)$
	1	$kg/m^3.s(at\ P_L)$
k_{ez}	0.293	$J/m.s.K$
h_o	40	$J/m^2.s.K$
t_o	54800	s
c_o	0.79	mol/m^3
T_o	303	K
v_H	0.25	m/s
v_L	0.5	m/s
P_H	5.07x10^5	Pa
P_L	1.01x10^5	Pa
α	2	–
t_1	$0.01t_o$	sec
t_2	$0.01t_o$	sec

Table 1. Physical data used in the model

is NLPQL by Schittkowski (1986) and VODE code is used as the integrator (Brown et al. (1989)). Appropriate changes are introduced in the dynamic optimisation package DYNO (Fikar and Latifi (2002)) for computation of gradients by adjoint system method for the hybrid dynamic system.

Table (2) presents the optimal values of the performance index, i.e. the CSS condition, and their corresponding CPU times for the two methods of gradients computation. It can be seen that adjoint system method has not only faster convergence rate but it also leads to a more precise value of the CSS condition.

	Finite differnces method	Adjoint system method
CPU time (s)	1505	62
Performance index	0.53x10^{-4}	0.49x10^{-5}

Table 2. PSA optimisation results

Figures (3), (4) and (5) present respectively the adsorbate concentration in fluid and solid phases and fluid phase temperature after the adsorption step versus dimensionless bed length at the end of first cycle and at CSS.

The results are in very good agreement with those obtained in (Chihara and Suzuki (1983)) where the complete discretisation based on Crank-Nicolson implicit method is used. However the computational time must be huge compared to the adjoint sytem method developed here.

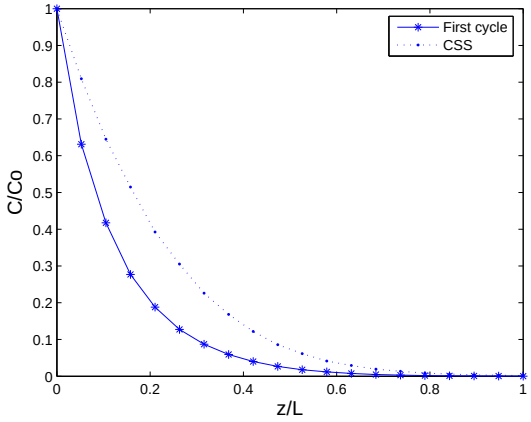

Figure 3. Fluid phase concentration profiles *vs* dimensionless bed length

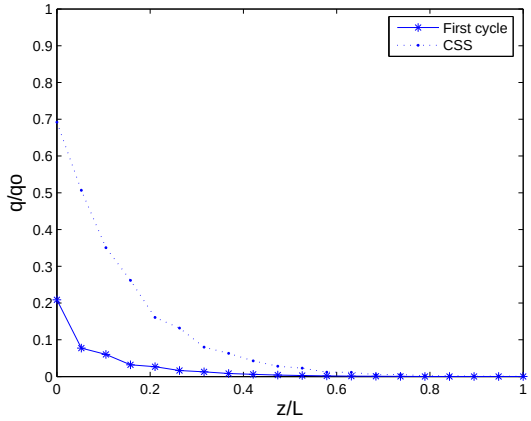

Figure 4. Solid phase concentration profiles *vs* dimensionless bed length

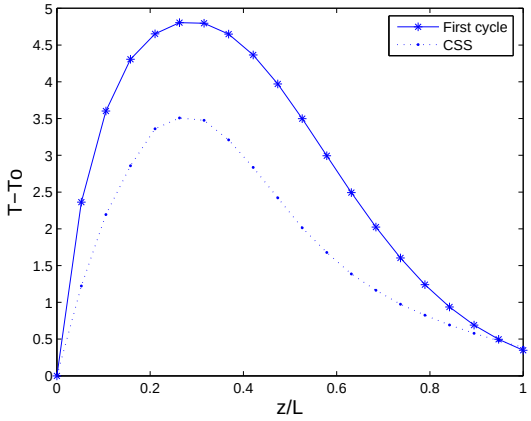

Figure 5. Fluid phase temperature profiles *vs* dimensionless bed length

8. CONCLUSION

Optimisation-based simulation of the hybrid PSA process was carried out by simultaneous treatment of simulation and optimisation as a single problem. The adjoint system for computation of gradients was formulated for the hybrid dynamic

model and the results were compared to finite differences method. It is clear that adjoint system method can be used for computation of gradients for hybrid dynamic optimisation problems and it gives better convergence rate.

Nomenclature

a_v	Interfacial surface area
c	Fluid-phase concentration
c_o	Adsorbate concentration in feed
C_{pg}	Heat capacity of gas
C_{ps}	Heat capacity of adsorbent
h_o	Overall heat transfer coeffcient
K	k/k_o
k	Adsorption equilibrium constant
k_o	k at T_o
k_{ez}	Effective thermal conductivity
K_s/γ	Overall mass transfer coefficient
L	Bed length
P_H	Adsorption step bed pressure
P_L	Purge step bed pressure
Q	Isosteric heat of adsorption
q	Solid-phase concentration
r	Radius of the adsorbent bed
T	Temperature in the bed
t	Time
T_o	Ambient temperature
t_o	Characteristic time/saturation time
v	Interstitial velocity
z	Position in the bed
$\bar{c}$	c/c_o
$\bar{q}$	q/q_o^*
$\bar{q}_o^*$	q^*/q_o^*
$\bar{T}$	$(T-T_o)/T$
$\bar{t}$	t/t_1
$\bar{z}$	z/L
α	Volumetric purge to feed ratio
ϵ	Bed porosity
γ	Bed density
ρ_g	Gas density
ρ_s	Adsorbent particle density

Nondimensional parameters

$$\tau_a = \frac{t_1 v}{L}$$
$$\tau_b = \frac{\gamma q_o^*}{\epsilon c_o}$$
$$\tau_f = \frac{t_1 K_s a_v}{\gamma}$$
$$\tau_H = \frac{\epsilon v \rho_g C_{pg} t_1}{L(\epsilon\rho_g C_{pg} + \gamma C_{ps})}$$
$$\tau_L = \frac{t_1 k_{ez}}{L^2(\epsilon\rho_g C_{pg} + \gamma C_{ps})}$$
$$\tau_W = \frac{t_1 2h_o}{r(\epsilon\rho_g C_{pg} + \gamma C_{ps})}$$
$$\beta = \frac{\gamma Q q_o^*}{T_o(\epsilon\rho_g C_{pg} + \gamma C_{ps})}$$

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