

Analysis of a one-component sorption in a single adsorbent particle by the orthogonal collocation method

II. Nonisothermal models

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In this paper the process of a nonisothermal one-component sorption in a single adsorbent particle is studied. Nine models of various complexity are described making it possible to calculate the transients of average values of dimensionless adsorbate concentration and dimensionless temperature rise in particle during an adsorption process. It is shown that in most practical cases the model can be used in which both film resistances and intraparticle resistance against mass transfer are included.

В этой статье разбирается процесс неизотермической однокомпонентной сорбции в одной частице адсорбента. Описывается девять моделей различной сложности, позволяющих рассчитать временные зависимости средней безразмерной концентрации адсорбированного вещества и безразмерного температурного повышения во время адсорбции. Указывается на то, что в большинстве практических случаев можно использовать модель, в которую включены сопротивления переходу вещества и теплоты в пленке и внутричастичное сопротивление по отношению к переходу вещества.

In the previous paper [1] we treated the isothermal models of a one-component sorption in a single adsorbent particle and presented some interesting features of orthogonal collocation solution results when compared with the exact results. The problem of nonisothermal sorption has recently attracted the attention of several authors [2—8]. A detailed analysis has been made by *Brunovská et al.* [5—8]. Their method of solution is apparently numerically satisfactory, but is not suited for practical use (for example in computation of packed bed adsorbers described by two phase models) because of a long computation time. It is the reason why we used the orthogonal collocation method for the solution of model equations.

Mathematical models

The basic model (mass and heat balances) for a nonisothermal one-component sorption in a single spherical adsorbent pellet may be formally derived from the differential mass and energy balances of the adsorptive in a stream of carrier gas [5, 9].

$$\varepsilon \frac{\partial c}{\partial t} = D_{ef} \left(\frac{\partial^2 c}{\partial x^2} + \frac{2}{x} \frac{\partial c}{\partial x} \right) - \frac{\partial a}{\partial t} \quad (1)$$

$$\rho C_p \frac{\partial T}{\partial t} = \lambda_{ef} \left(\frac{\partial^2 T}{\partial x^2} + \frac{2}{x} \frac{\partial T}{\partial x} \right) + (-\Delta H_{ad}) \frac{\partial a}{\partial t} \quad (2)$$

The two transport coefficients D_{ef} and λ_{ef} which are considered to be constant are composite properties that reflect the different transport mechanisms inside the complex pore structure. The initial and boundary conditions are

$$\begin{aligned} a &= a_i \\ c &= c_i^* \quad \text{at } 0 \leq x \leq R \quad \text{for } t=0 \\ T &= T_i \end{aligned} \quad (3)$$

$$\frac{\partial c}{\partial x} = \frac{\partial T}{\partial x} = 0 \quad \text{at } x=0 \quad \text{for } t>0 \quad (4)$$

$$\frac{\partial c}{\partial x} = \frac{h_M}{D_{ef}} (c_b - c_{x=R}) \quad (5a)$$

at $x=R$ for $t>0$

$$\frac{\partial T}{\partial x} = \frac{h}{\lambda_{ef}} (T_b - T_{x=R}) \quad (5b)$$

T_b and c_b being properties of the bulk fluid phase; T_b and c_b are generally functions of position in the reactor and of time. We shall regard them as known constant values $c_b = c_0$ and $T_b = T_i \cdot h_M$ and h are mass and heat transfer coefficients for the film that surrounds the pellet. Eqns (1–5) may be rendered dimensionless by the following substitutions [5]

$$\begin{aligned} q &= \frac{a - a_i}{a_i^* - a_i} & Q &= \frac{c - c_i^*}{c_0 - c_i} & \tau &= \frac{c_0 - c_i^*}{a_i^* - a_i} \frac{D_{ef} t}{R^2} \\ \Theta &= \frac{\rho C_p \Delta T}{(-\Delta H_{ad})(a_i^* - a_i)} & \delta &= \frac{\varepsilon(c_0 - c_i^*)}{a_i^* - a_i} & \xi &= \frac{x}{R} \\ Lw &= \frac{\lambda_{ef}(a_i^* - a_i)}{\rho C_p D_{ef}(c_0 - c_i^*)} & Bi_M &= \frac{h_M R}{D_{ef}} & Bi &= \frac{h R}{\lambda_{ef}} \end{aligned} \quad (6)$$

to obtain

$$\delta \frac{\partial Q}{\partial \tau} = \nabla^2 Q - \frac{\partial q}{\partial \tau} \quad (7)$$

$$\frac{\partial \Theta}{\partial \tau} = Lw \nabla^2 \Theta + \frac{\partial q}{\partial \tau} \quad (8)$$

The initial and boundary conditions are

$$\begin{aligned} q &= 0 \\ Q &= 0 \quad \text{at } 0 \leq \xi \leq 1 \quad \text{for } \tau = 0 \\ \Theta &= 0 \end{aligned} \quad (9)$$

$$\frac{\partial Q}{\partial \xi} = \frac{\partial \Theta}{\partial \xi} = 0 \quad \text{at } \xi = 0 \quad \text{for } \tau > 0 \quad (10)$$

$$\frac{\partial Q}{\partial \xi} = Bi_M(1 - Q_{\xi=1}) \quad \text{at } \xi = 1 \quad \text{for } \tau > 0 \quad (11a)$$

$$\frac{\partial \Theta}{\partial \xi} = -Bi \Theta_{\xi=1} \quad (11b)$$

For the Langmuir isotherm

$$a = a_s \frac{Kp}{1 + Kp} \quad (12)$$

and using transformations (6) and the following transformations

$$\begin{aligned} \kappa_1 &= \frac{a_s^* - a_i}{a_s - a_i} & \kappa_2 &= \frac{a_i(a_s - a_s^*)}{a_s(a_s^* - a_i)} \\ \alpha &= \frac{(-H_{ad})}{RT_i} & \beta &= \frac{(-\Delta H_{ad})}{\rho C_p T_i} (a_s^* - a_i) \end{aligned} \quad (13)$$

we obtain

$$Q = \left[\frac{(1 - \kappa_1)q}{1 - \kappa_1 q} + \kappa_2 \right] \frac{1}{1 + \beta \Theta} \exp \frac{\alpha \beta \Theta}{1 + \beta \Theta} - \kappa_2 \quad (14)$$

The governing eqns (7–11) and (14) are represented by a set of strongly nonlinear coupled parabolic differential equations which are coupled to the fluid phase mass and energy balances through boundary conditions (11a, 11b). This complicated model, however, is difficult to treat numerically and one is interested in using a model which is as simple as possible. In describing most sorption processes, intraparticle temperature gradients may be neglected [8]. We integrate (8) over the pellet volume to obtain

$$\frac{d\bar{\Theta}}{d\tau} = 3Lw \left(\frac{\partial \Theta}{\partial \xi} \right)_{\xi=1} + 3 \int_0^1 \frac{\partial q}{\partial \tau} \xi^2 d\xi \quad (15)$$

the boundary condition (11b) which contains unknown temperature $\Theta_{\xi=1}$ can be used in the modified form

$$\left(\frac{\partial \Theta}{\partial \xi} \right)_{\xi=1} = -\bar{Bi}\bar{\Theta} \quad (16)$$

Villadsen and Michelsen [9] recommended to compensate, for the use of larger temperature driving force by using a smaller value of \bar{Bi}

$$\bar{Bi} = \frac{Bi}{1 + 0.2Bi} \quad (17)$$

Eqn (16) is inserted into (15) to give a simplified form of heat balance

$$\frac{d\bar{\Theta}}{d\tau} = -3Lw\bar{Bi}\bar{\Theta} + 3 \int_0^1 \frac{\partial q}{\partial \tau} \xi^2 d\xi \quad (18)$$

Some further simplification of the model is possible for large values of film transfer coefficients. These are equivalent to small changes in driving forces across the film. Boundary conditions (11a) and (11b) for large Bi_M and Bi , respectively, have the form

$$Q_{\xi=1} = 1 \quad (19a)$$

$$\Theta_{\xi=1} = 0 \quad \text{at } \xi = 1 \quad \text{for } \tau \geq 0 \quad (19b)$$

Table 1 lists mathematical formulations of nine different models, which can be obtained by the application of various simplifications. Model N1, in which all transport resistances are included, is the most complicated. In model N2 only the intraparticle transport resistances are included and in N3 only the film resistances against the heat and mass transport are dominant. In models N4—N9 various combinations of transport resistances inside the particle and in the film, respectively, are included.

Analysis of the nonisothermal models

All models listed in Table 1 are represented by the set of two strongly nonlinear coupled differential equations. They need to be solved numerically. An approximate analysis based on a linear driving force representation of the mass transfer rate equation was developed by Chihara *et al.* [2], while a solution in terms of the moments of the uptake curves was obtained by Kočířík *et al.* [3]. Brunovská *et al.* solved, in recent papers, some models from Table 1 [5—8]. In paper [5] a detailed

Table 1

Mathematical formulations of nine nonisothermal models

Model	Model equations	Boundary conditions
N1		$\nabla Q(1) = Bi_m(1 - Q(1))$ $\nabla \Theta(1) = -Bi\Theta(1)$
N2	$\delta \frac{\partial Q}{\partial \tau} = \nabla^2 Q - \frac{\partial q}{\partial \tau}$	$Q(1) = 1$ $\Theta(1) = 0$
N4	$\frac{\partial \Theta}{\partial \tau} = Lw\nabla^2 \Theta + \frac{\partial q}{\partial \tau}$	$\nabla Q(1) = Bi_m(1 - Q(1))$ $\Theta(1) = 0$
N5		$Q(1) = 1$ $\Theta(1) = -Bi\Theta(1)$
N6	$\frac{\partial Q}{\partial \tau} = \nabla^2 Q - \frac{\partial q}{\partial \tau}$	$\nabla Q(1) = Bi_m(1 - Q(1))$ $\nabla \Theta(1) = -Bi\bar{\Theta}$
N8	$\frac{d\bar{\Theta}}{d\tau} = 3Lw\left(\frac{\partial \Theta}{\partial \xi}\right)_{\xi=1} + 3 \int_0^1 \frac{\partial q}{\partial \tau} \xi^2 d\xi$	$Q(1) = 1$ $\nabla \Theta(1) = -Bi\bar{\Theta}$
N7	$\frac{d\bar{Q}}{d\tau} = 3\left(\frac{\partial Q}{\partial \xi}\right)_{\xi=1} - 3 \int_0^1 \frac{\partial q}{\partial \tau} \xi^2 d\xi$	$\nabla Q(1) = \bar{Bi}_m(1 - \bar{Q})$ $\nabla \Theta(1) = -Bi\Theta(1)$
N9	$\frac{\partial \Theta}{\partial \tau} = Lw\nabla^2 \Theta + \frac{\partial q}{\partial \tau}$	$\nabla Q(1) = \bar{Bi}_m(1 - \bar{Q})$ $\Theta(1) = 0$
N3	$\frac{\partial \bar{Q}}{\partial \tau} = 3\left(\frac{\partial Q}{\partial \xi}\right)_{\xi=1} - \frac{dq}{d\tau}$ $\frac{d\bar{\Theta}}{d\tau} = 3Lw\left(\frac{\partial \Theta}{\partial \xi}\right)_{\xi=1} + \frac{dq}{d\tau}$	$\nabla Q(1) = \bar{Bi}_m(1 - \bar{Q})$ $\nabla \Theta(1) = -\bar{Bi}\bar{\Theta}$

analysis of N2 is presented. A finite-difference method based on explicit-implicit procedure is proposed to approximate this set of equations. The equations are solved for a case of strong adsorption accompanied by significant heat generation effects. It is shown that for molecular diffusion intraparticle temperature differences may be of the order of magnitude 10–50°C. The next paper [6] is concerned with an analysis of N5 with finite values of film transfer coefficient for heat transport. For higher values of Bi overheating of the particle occurs, which is followed by a cooling process. On the other hand, for low values of Bi , the particle behaves “isothermally” and for a long time the temperature inside the particle does not change. The high temperature of the particle results in a slow adsorption process. In paper [7] an approximation is described making it possible to calculate temporal temperature and adsorbed amount profiles during an adsorption process in a single pellet for N8. The profiles calculated from models N8 and N5 are compared and it is shown that, for a majority of operating systems, the simplified

model can be used and approximates very well the results obtained from the exact model N5. An experimental study has been made of temperature profiles incident within a zeolite adsorbent particle in the course of adsorption of *n*-heptane [8]. The results of this work indicate that the overheating of an adsorbent particle is a very rapid process which is followed by a slow cooling of the hot particle. Experimental data are compared with predictions calculated from model N8. A numerical analysis of models [4—7] as well as experimental observations [4, 8] indicated that for many practical problems the internal diffusion resistance will dominate the external film resistance for mass transfer, whereas the external film resistance will dominate the internal resistance for heat transfer. Under certain conditions the internal and external resistances in the mass transport may be of equal magnitude.

Solution and computing methods

In the previous paper [1] the method of orthogonal collocation has been used for the solution of isothermal models in connection with the Runge—Kutta—Merson technique to solve the resulting ordinary differential equations. In this paper the same solution and computing methods are being used to solve the set of differential equations of N6 and N8. The heat balance in N6 and N8 has the form (18) and for a small value ($\delta = 0.00012$ in experimental conditions in [8]) it can be rewritten as

$$\frac{d\bar{\Theta}}{d\tau} = -3Lw\bar{Bi}\bar{\Theta} + 3\left(\frac{\partial Q}{\partial \xi}\right)_{\xi=1} \quad (20)$$

which is the form of the heat balance from [7]. For the equilibrium isotherm $q = q(Q, \bar{\Theta})$ we obtain

$$\left(\frac{\partial q}{\partial Q} + \delta\right)\frac{\partial Q}{\partial \tau} = \nabla^2 Q - \frac{\partial q}{\partial \bar{\Theta}} \frac{d\bar{\Theta}}{d\tau} \quad (21)$$

Model equations (20, 21) with boundary condition (11a) or (19a) respectively can be transformed by using formulas for the gradient ∇ and for the Laplace operator ∇^2 [9]

$$\nabla Q(I) = \sum_{J=1}^{N+1} A(I, J) Q(J) \quad (22)$$

$$\nabla^2 Q(I) = \sum_{J=1}^{N+1} B(I, J) Q(J) \quad (23)$$

into the form

$$f(Q(I), \bar{\Theta}) \frac{dQ(I)}{d\tau} = \sum_{J=1}^{N+1} B(I, J) Q(J) - g(Q(I), \bar{\Theta}) \frac{d\bar{\Theta}}{d\tau} \quad (24)$$

$$I = 1, \dots, N$$

and

$$Bi_M(1 - Q(N+1)) = \sum_{J=1}^{N+1} A(N+1, J) Q(J) \quad (25a)$$

or

$$Q(N+1) = 1 \quad (25b)$$

The unknown boundary ordinate is eliminated from the system of equations by the equation

$$Q(N+1) = - \frac{\sum_{J=1}^{N+1} A(N+1, J) Q(J)}{Bi_M + A(N+1, N+1)} + \frac{Bi_M}{Bi_M + A(N+1, N+1)} \quad (26)$$

which is inserted into each of eqns (24). Thus we obtain a system of N equations for the N interior values of Q and the mean temperature of the pellet

$$\frac{d\mathbf{Q}}{d\tau} = \mathbf{F}_1(\mathbf{Q}, \bar{\Theta}) \quad (27)$$

Eqn (20) can be rewritten, by using formulas (22) and (26), into the symbolic form

$$\frac{d\bar{\Theta}}{d\tau} = \mathbf{F}(\mathbf{Q}, \bar{\Theta}) \quad (28)$$

Eqns (27, 28) represent the set of the $N+1$ ordinary differential equations which are solved under the initial conditions

$$\begin{aligned} \mathbf{Q} &= 0 \\ \bar{\Theta} &= 0 \end{aligned} \quad \text{at } \tau = 0 \quad (29)$$

The set of ordinary differential equations was integrated by the Runge—Kutta—Merson method. The transients of the mean internal concentrations in both phases \bar{Q} and \bar{q} , respectively, were obtained by the Radau quadrature summation formula

$$\begin{aligned} \bar{Q} &= \sum_{I=1}^{N+1} W(I) Q(I) \\ \bar{q} &= \sum_{I=1}^{N+1} W(I) q(I) \end{aligned} \quad (30)$$

where $q(I) = q(Q(I), \bar{\Theta})$.

Elements $A(I, J)$, $B(I, J)$, $W(I)$ were computed by the programs listed in [9]. In this case the weighting function $(1 - \xi^2)^\alpha \xi^{2\beta}$ with $\alpha = 0$ and $\beta = 1/2$ has been used. The approximation order N of the orthogonal polynomials was tested with $N = 1, 2, \dots, 7, 8$. $N = 7$ proved to be sufficient to obtain differences only in the 4th

digit as compared with the higher approximation. The method of orthogonal collocation in connection with the Runge—Kutta—Merson technique was compared with an explicit-implicit finite difference method from [7] for model N6. For the same degree of accuracy ($N=7$) less than 1/20th of the computation time was required. The use of a more sophisticated integration technique would have permitted larger time steps and produced results even more favourable to the collocation technique.

Results and discussion

Computation results are plotted in Figs. 1—4. In Figs. 1—3 some transients of average values of dimensionless sorbate concentration in particle \bar{q} , dimensionless gaseous phase concentration \bar{Q} , and of dimensionless temperature of particle are drawn for various values of parameter Bi_M for model N6. Solutions are compared with the solution of N8 for the same parameters. The differences between both models are significant only for low values of Bi_M . For $20 < Bi_M < 20\,000$ within which one will normally expect parameter values to be within physically realistic conditions the differences between both models are small. The measured concen-

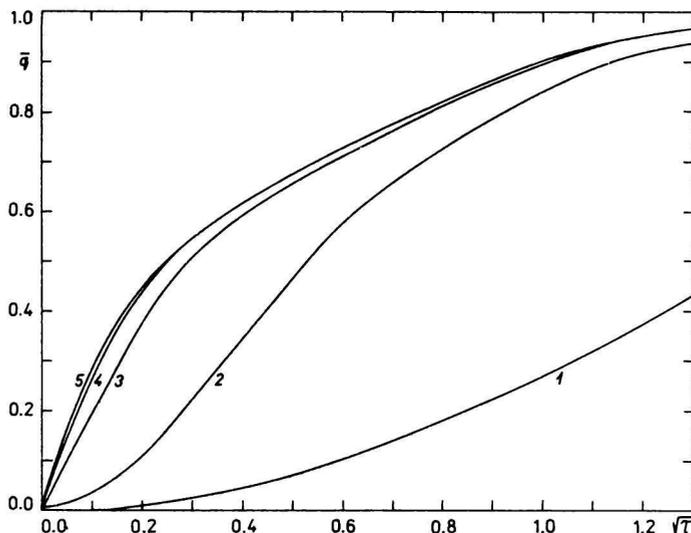


Fig. 1. Transients of \bar{q} for models N6 and N8.

$\kappa_1 = 0.7$; $\beta = 0.3$; $\alpha = 10$; $\delta = 0.05$; $\omega = 3$.

1, 2, 3, 4. Model N6; 5. model N8.

1. $Bi_M = 0.1$; 2. $Bi_M = 1$; 3. $Bi_M = 10$; 4. $Bi_M = 100$.

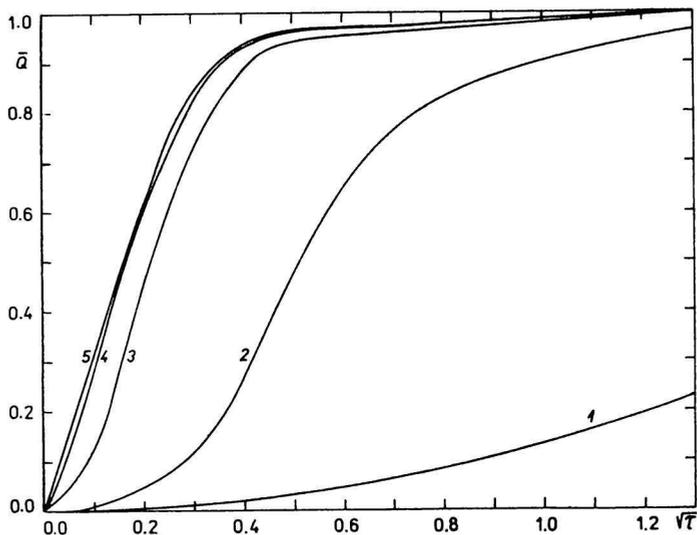


Fig. 2. Transients of \bar{Q} for models N6 and N8.

$$\kappa_1 = 0.7; \beta = 0.3; \alpha = 10; \delta = 0.05; \omega = 3.$$

1, 2, 3, 4. Model N6; 5. model N8.

1. $Bi_M = 0.1$; 2. $Bi_M = 1$; 3. $Bi_M = 10$; 4. $Bi_M = 100$.

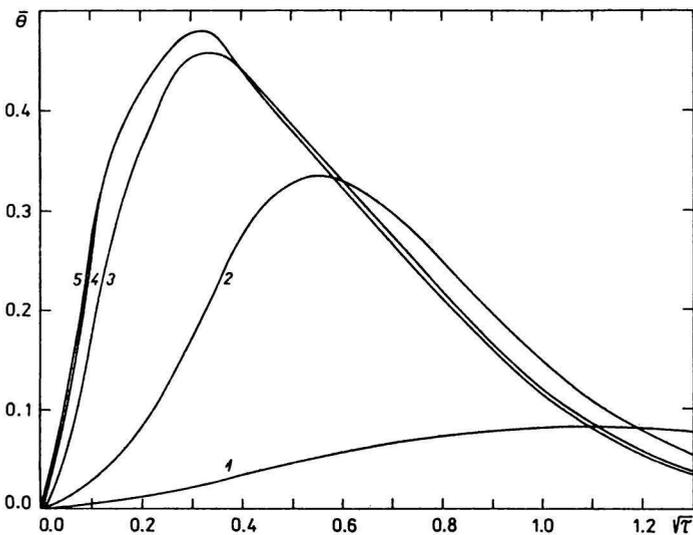


Fig. 3. Transients of $\bar{\Theta}$ for models N6 and N8.

$$\kappa_1 = 0.7; \beta = 0.3; \alpha = 10; \delta = 0.05; \omega = 3.$$

1, 2, 3, 4. Model N6; 5. model N8.

1. $Bi_M = 0.1$; 2. $Bi_M = 1$; 3. $Bi_M = 10$; 4. $Bi_M = 100$.

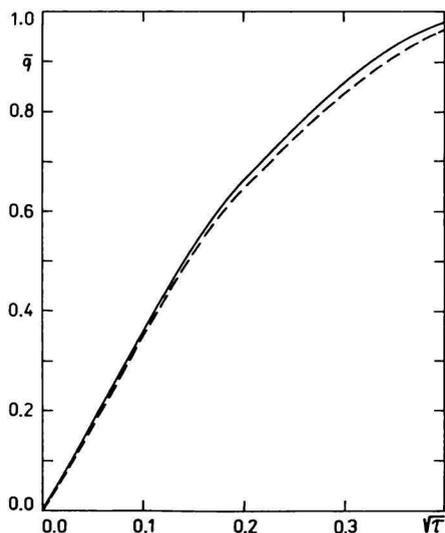


Fig. 4. Transients of \bar{q} for models I2 and N8.
 — Isothermal model I2, $\delta = 0.00012$, $\kappa_1 = 0.908$;
 - - - nonisothermal model N8, $\delta = 0.00012$,
 $\kappa_1 = 0.908$, $\omega = 25$, $\alpha = 14.37$, $\beta = 0.157$.

tration transients from [8] are drawn in Fig. 4 together with computed results for parameters recommended in [8] for nonisothermal model N8 and those for isothermal model I2 from [1]. From Fig. 4 it is evident that the concentration dependence in the particle may be computed with relative deviation less than 6% by the isothermal model.

Conclusion

Computation showed that the orthogonal collocation method is also suitable for solving mathematical models of nonisothermal one-component sorption. Conclusions about collocation solution accuracy are quite similar to those obtained with isothermal nonlinear models [1]. From the figures presented in this paper it may be deduced: 1. the major mass transport resistance is distributed as diffusional resistance inside the pellet; 2. the high thermal effects have only little influence on the concentration transient for parameters presented here.

Finally we can say that the most sophisticated model for one-component sorption in a single particle is N6, in which both film resistance and intraparticle resistance against mass transport are included. In most practical cases the less general model N8 is also good though it is hardly less complicated than model N6 from the mathematical and data points of view. When one is interested only in concentration transient, or when a priori estimation of parameters Bi and Lw is complicated, isothermal models I1 or I2 from [1] can be used with accuracy, satisfactory for chemical engineering problems, for parameters presented here.

Symbols

a	adsorbate concentration in particle	mol m^{-3}
a_i	initial adsorbate concentration in particle	mol m^{-3}
a_s	monolayer capacity in the Langmuir isotherm	mol m^{-3}
a_0^*	equilibrium adsorbate concentration	mol m^{-3}
$A(I, J)$	differentiation weight from eqn (22)	
$B(I, J)$	differentiation weight from eqn (23)	
$\frac{Bi}{Bi}$	Biot number for heat transfer	
$\frac{Bi_M}{Bi_M}$	modified Bi defined by eqn (17)	
$\frac{Bi_M}{Bi_M}$	Biot number for mass transfer	
$\frac{Bi_M}{Bi_M}$	modified Bi_M defined by eqn (17)	
c	adsorptive concentration in the gaseous phase	mol m^{-3}
c_b	adsorptive concentration in the bulk flow	mol m^{-3}
c_i^*	equilibrium initial adsorptive concentration	mol m^{-3}
$c_{x=R}$	adsorptive concentration at the particle surface	mol m^{-3}
c_0	constant adsorptive concentration in the bulk flow	mol m^{-3}
C_p	specific heat of sorbent	$\text{J kg}^{-1} \text{K}^{-1}$
D_{ef}	effective diffusivity	$\text{m}^2 \text{s}^{-1}$
f, g	functions from eqn (24)	
F	function from eqn (28)	
F_1	vector of functions from eqn (27)	
h	film heat transfer coefficient	$\text{J m}^{-2} \text{s}^{-1} \text{K}^{-1}$
h_M	film mass transfer coefficient	m s^{-1}
$(-H_{ad})$	heat of adsorption	J mol^{-1}
K	equilibrium parameter in the Langmuir equation	Pa^{-1}
LW	modified Lewis number	
N	number of internal collocation points	
p	partial pressure of adsorptive	Pa
q	dimensionless adsorbate concentration in particle	
\bar{q}	average dimensionless adsorbate concentration	
Q	dimensionless adsorptive concentration in the gaseous phase	
\bar{Q}	average dimensionless adsorptive concentration	

$Q_{\xi=1} = Q(1) = Q(N+1)$	dimensionless concentration at the particle surface	
$Q(I)$	dimensionless concentration at I -th collocation point	
Q	column vector with $Q(I)$ elements	
R	radius of particle	m
\mathcal{R}	gas constant	$\text{J mol}^{-1} \text{K}^{-1}$
t	time	s
T	temperature	K
T_i	initial temperature	K
T_b	temperature in the bulk flow	K
T_{1-R}	temperature at the particle surface	K
$W(I)$	Radau quadrature weight from eqn (30)	
x	space coordinate	m
α	dimensionless adsorption energy	
β	dimensionless adiabatic temperature rise	
δ	dimensionless parameter defined by eqn (6)	
ε	porosity of particle	
Θ	dimensionless temperature rise	
$\Theta_{\xi=1} = \Theta(1)$	dimensionless temperature rise at the particle surface	
$\bar{\Theta}$	average dimensionless temperature rise	
κ_1, κ_2	dimensionless parameters defined by eqn (13)	
λ_{cr}	effective thermal conductivity of sorbent particle	$\text{J m}^{-1} \text{s}^{-1} \text{K}^{-1}$
ρ	density of sorbent particle	kg m^{-3}
ξ	dimensionless space coordinate	
τ	dimensionless time	

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