

Modelling of catalytic reactors with catalyst deactivation

III. Pseudohomogeneous model of reactor with axial dispersion

M. BARTO, A. BRUNOVSKÁ, and J. ILAVSKÝ

*Department of Organic Technology, Slovak Technical University,
CS-812 37 Bratislava*

Received 21 May 1984

Accepted for publication 10 December 1985

In this paper a pseudohomogeneous model of fixed bed catalytic reactor with axial dispersion is described. The conception of this model is based on the assumption that the catalyst is deactivated by irreversible chemisorption of catalyst poison. An algorithm for solution of the system of model equations as well as a comparison of numerical results with experimental ones and with the model of well-mixed regions in series is also presented.

В работе описана псевдогомогенная модель с аксиальной дисперзией каталитического реактора с неподвижным слоем катализатора и дезактивацией катализатора, которая применена необратимой хемисорпцией каталитического яда. Она содержит алгоритм решения системы уравнений модели и сравнение экспериментальных данных с численными результатами и тоже сравнение с моделью каскады смешанных областей.

The problem of deactivation of catalyst belongs among principal problems which are to be solved in connection with design of fixed bed catalytic reactors. A decrease in activity of catalyst leads to a decrease of the performance of the reactor. There are concentration and temperature profiles which move downstream through the reactor and vanish with total deactivation. At a certain degree of deactivation, when the performance of reactor is very small, the reactor has to be set aside and the catalyst is to be regenerated or replaced by a new one. A design of such catalytic reactor, its operation regime as well as investigation of its dynamic properties requires an adequate mathematical model.

In our preceding papers [1, 2] we have described two pseudohomogeneous models of fixed bed catalytic reactor in which the catalyst is deactivated by irreversible chemisorption of catalyst poison, *i.e.* the model with plug-flow and the model of well-mixed regions in series. A more detailed description has been given by the model of well-mixed regions in series [2] which is consistent with the concentrations of reaction components and catalyst poison at the exit from reactor and qualitatively fairly describes the advance of temperature wave through reactor (good accordance of maximum temperature). However, the shape of temperature

wave does not correspond with experiment. This is why we present a one-dimensional pseudohomogeneous model with axial dispersion.

The model of fixed bed reactor with axial dispersion has been presented in papers [3, 4]. However, the first studies in which this model is applied in connection with deactivation of catalyst are described in papers [5–7].

As for recent communications, we must mention the papers by *Do* and *Weiland* [8, 9] who used the perturbation method for deriving explicit formulas which could be applied to calculation of the isothermal concentration profile of reactant for parallel and consecutive deactivation in a tube reactor with axial dispersion.

The aim of this study has been to compare the model with axial dispersion with the models described earlier [1, 2] as well as with experiment and to propose an effective method for solving the system of model equations.

Pseudohomogeneous model with axial dispersion

Provided the deactivation of catalyst due to irreversible chemisorption of catalyst poison (which is present as impurity in the feed) takes place, the one-dimensional pseudohomogeneous model of catalytic reactor with axial dispersion [3, 4] is to be described by the following system of equations

$$\varepsilon \frac{\partial c_B}{\partial t} + v \frac{\partial c_B}{\partial z} - D_B \frac{\partial^2 c_B}{\partial z^2} - v_B Q_b \dot{\xi}_w = 0 \quad (1)$$

(mass balance of key component)

$$\varepsilon \frac{\partial c_j}{\partial t} + v \frac{\partial c_j}{\partial z} - D_j \frac{\partial^2 c_j}{\partial z^2} + Q_b \frac{\partial a_j}{\partial t} = 0 \quad (2)$$

(mass balance of catalyst poison)

$$\bar{c}_p \frac{\partial T}{\partial t} + v Q_b c_{PB} \frac{\partial T}{\partial z} - \lambda_1 \frac{\partial^2 T}{\partial z^2} - (-H) Q_b v_b \dot{\xi}_w + \frac{4h}{d_t} (T - T_c) = 0 \quad (3)$$

(enthalpy balance)

$$\dot{\xi}_w = f(c_i, T) \cdot h(a_j) \quad (4)$$

(kinetic equation of catalytic reaction)

$$\frac{da_j}{dt} = g(c_j, T, a_j) \quad (5)$$

(rate equation of chemisorption of catalyst poison)

$$z = 0: v(c_{B0} - c_B) = -D_B \frac{\partial c_B}{\partial z}$$

$$v(c_{j0} - c_j) = -D_j \frac{\partial c_j}{\partial z} \quad (6)$$

$$v \rho_g c_{pB} (T_0 - T) = -\lambda_1 \frac{\partial T}{\partial z}$$

$$z = L: \frac{\partial c_B}{\partial z} = \frac{\partial c_J}{\partial z} = \frac{\partial T}{\partial z} = 0 \quad (7)$$

(boundary conditions)

$$t = 0: \quad 0 \leq z \leq L, \quad a_j = 0$$

$$v \frac{\partial c_B}{\partial z} - D_B \frac{\partial^2 c_B}{\partial z^2} - v_B \rho_b \xi_w = 0$$

$$v \frac{\partial c_J}{\partial z} - D_J \frac{\partial^2 c_J}{\partial z^2} + \rho_b \frac{\partial a_J}{\partial t} = 0 \quad (8)$$

$$v \rho_g c_{pB} \frac{\partial T}{\partial z} - \lambda_1 \frac{\partial^2 T}{\partial z^2} - (-H) v_B \rho_b \xi_w + \frac{4h}{d_t} (T - T_c) = 0$$

(initial conditions)

The initial conditions involve the assumption that the poison started entering into reactor at the time moment $t=0$, *i.e.* no poison was present in the layer at the beginning of the process and the concentration profiles as well as the temperature profile corresponded to the reaction on fresh catalyst.

The system of model equations (1–8) is valid under the following conditions:

Only one catalytic reaction and one deactivation process occur. The rate of deactivation is independent of the rate of catalytic reaction.

The catalytic rate equation is separable [1].

The dependence of activity of catalyst ϕ on the adsorbed amount of the poison is linear; $\phi = (a_j^* - a_j)/a_j^*$.

Constant concentrations and temperature profile of a certain shape (*e.g.* parabola) are assumed to be in each cross-section of reactor, *i.e.* the radial dispersion may be neglected.

There is a perfect heat exchange between gas and catalyst.

The density of reaction mixture is constant.

The specific heats of reacting substances and catalyst, reaction heat, diffusion coefficients and coefficient of heat conduction in axial direction are independent of temperature.

The amount of the reactant adsorbed on active centres of catalyst is negligible.

The amount of heat released by chemisorption of the poison is negligible with respect to reaction heat.

The last assumption results from the fact that the poison is present only in small amounts and its concentration is considerably lower than the concentration of the key component.

By introducing dimensionless variables

$$\begin{aligned} Z &= \frac{Q_b \xi_w^0 z}{c_{B0} v} & A_J &= \frac{a_J}{a_J^*} \\ \tau &= \frac{t}{t^0} & \Theta &= \frac{T - T_0}{T_{ad}} \\ Y_B &= \frac{c_B}{c_{B0}} & \Theta_c &= \frac{T_c - T_0}{T_{ad}} \\ Y_J &= \frac{c_J}{c_{J0}} & \dot{\Xi} &= \frac{\dot{\xi}_w}{\xi_w^0} \end{aligned} \quad (9)$$

and parameters

$$\begin{aligned} \delta &= \frac{\varepsilon c_{B0}}{Q_b \xi_w^0 t^0} & G &= \frac{c_{B0} a_J^*}{\xi_w^0 t^0 c_{J0}} \\ R_s &= \frac{\overline{Q_c} c_{B0}}{Q_g c_{pg} Q_b \xi_w^0 t^0} & F &= \frac{4h c_{B0}}{d_t Q_b \xi_w^0 Q_g c_{pg}} \\ Pe_B &= \frac{vL}{D_B} & Pe_J &= \frac{vL}{D_J} & Pe_h &= \frac{vL Q_g c_{pg}}{\lambda_t} \end{aligned} \quad (10)$$

we obtain balance equations (1—3) in dimensionless form

$$\delta \frac{\partial Y_B}{\partial \tau} + \frac{\partial Y_B}{\partial Z} - \frac{1}{Pe_B} \frac{\partial^2 Y_B}{\partial Z^2} - v_B \dot{\Xi} = 0 \quad (11)$$

$$\delta \frac{\partial Y_J}{\partial \tau} + \frac{\partial Y_J}{\partial Z} - \frac{1}{Pe_J} \frac{\partial^2 Y_J}{\partial Z^2} - G \frac{\partial \phi}{\partial \tau} = 0 \quad (12)$$

$$R_s \frac{\partial \Theta}{\partial \tau} + \frac{\partial \Theta}{\partial Z} - \frac{1}{Pe_h} \frac{\partial^2 \Theta}{\partial Z^2} + v_B \dot{\Xi} + F(\Theta - \Theta_c) = 0 \quad (13)$$

The rate equations of catalytic reaction and chemisorption of poison (4) and (5) assume the form

$$\dot{\Xi} = \dot{\Xi}(Y_i, \Theta) \cdot \gamma(A_J) \quad (14)$$

$$-\frac{d\phi}{d\tau} = \frac{dA_J}{d\tau} = \varphi(Y_J, \Theta, A_J) \quad (15)$$

The boundary and initial conditions (6—8) transform in

$$Z = 0: \frac{\partial Y_B}{\partial Z} = Pe_B(Y_B - 1)$$

$$\frac{\partial Y_J}{\partial Z} = Pe_J(Y_J - 1) \quad (16)$$

$$\frac{\partial \Theta}{\partial Z} = Pe_h \Theta$$

$$Z = Z_L: \frac{\partial Y_B}{\partial Z} = \frac{\partial Y_J}{\partial Z} = \frac{\partial \Theta}{\partial Z} = 0 \quad (17)$$

$$\tau = 0: Z \geq 0; A_J = 0 \quad (18)$$

$$\frac{\partial Y_B}{\partial Z} - \frac{1}{Pe_B} \frac{\partial^2 Y_B}{\partial Z^2} - v_B \dot{\Xi} = 0 \quad (19)$$

$$\frac{\partial Y_J}{\partial Z} - \frac{1}{Pe_J} \frac{\partial^2 Y_J}{\partial Z^2} - G \frac{\partial \phi}{\partial \tau} = 0 \quad (20)$$

$$\frac{\partial \Theta}{\partial Z} - \frac{1}{Pe_h} \frac{\partial^2 \Theta}{\partial Z^2} + v_B \dot{\Xi} + F(\Theta - \Theta_c) = 0 \quad (21)$$

If the rate of deactivation is considerably smaller than the rate of catalytic reaction, the derivatives of concentrations and temperature with respect to time in balance equations (11–13) may be neglected, which means that a quasi-steady state is assumed. Then the system of the model equations is given by eqns (19–21).

Experimental

The experiment is fully described in papers [1, 2]. In order to facilitate the comprehension of reader, we describe it shortly in this communication, too.

The reactor was composed of two coaxial tubes and the bed of catalyst was placed between two layers of glass balls (approximately of equal size as the particles of catalyst) in the internal tube. The external tube formed a jacket and served for heating with streaming silicone oil. A capillary with moving thermocouple for measuring the temperature profile was placed in the reactor axis. The length of reactor was 0.9 m, internal diameter 0.0164 m, and external diameter of capillary with thermocouple 0.0041 m.

The hydrogenation of benzene on nickel catalyst (Ni on alumina, $w_{Ni} = 0.58$) with thiophene as catalyst poison was chosen again as model reaction. The catalyst was activated immediately in the reactor for 8 h at the temperature of 180 °C and at the hydrogen flow of 80 cm³ min⁻¹. After finishing the activation, the reactor was cooled to working temperature and a stream of benzene and hydrogen was

introduced into the reactor. As soon as the conditions were established, the entering stream was switched to the stream containing thiophene. In the course of measurement, the composition of outlet stream was determined by gas chromatography and the temperature found in the reactor axis was used for calculating the mean temperature in a given cross-section on the assumption of parabolic profile.

The conditions of the measurements presented in this paper are:

Particle size of catalyst: mesh fraction between 1.25 and 1.40 mm.

Mass of catalyst: 15.0065 g

Temperature at the inlet into the catalytic layer: 99.1 °C

Temperature of jacket: 99.1 °C

Volumetric flow: $2.38 \times 10^{-6} \text{ m}^3 \text{ s}^{-1}$

Input concentration of benzene: 1.89 mol m^{-3}

Input concentration of thiophene: $6.17 \times 10^{-2} \text{ mol m}^{-3}$

The rate of this catalytic reaction is [1, 2]

$$\dot{\xi}_{\text{sw}} = \phi \frac{k_{\infty} K_{\infty} p_{\text{B}} p_{\text{H}} \exp [-(Q+E)/RT]}{1 + K_{\infty} p_{\text{B}} \exp (-Q/RT)} \quad (22)$$

or in dimensionless form

$$\dot{\xi} = \phi \frac{(1 + \kappa_{\text{B}}) Y_{\text{B}} Y_{\text{H}} \exp [(\alpha_{\text{i}} + \alpha_{\text{K}}) \beta \Theta / (1 + \beta \Theta)]}{1 + \kappa_{\text{B}} Y_{\text{B}} \exp [\alpha_{\text{K}} \beta \Theta / (1 + \beta \Theta)]} \quad (23)$$

where

$$\begin{aligned} \kappa_{\text{B}} &= K_{\infty} p_{\text{B}0} \exp (-Q/RT_0) \\ \alpha_{\text{i}} &= E/RT_0 \\ \alpha_{\text{K}} &= Q/RT_0 \\ \beta &= T_{\text{ad}}/T_0 \end{aligned} \quad (24)$$

$$\dot{\xi}_{\text{sw}}^{\circ} = \frac{k_{\infty} K_{\infty} p_{\text{B}0} p_{\text{H}0} \exp [-(Q+E)/RT_0]}{1 + K_{\infty} p_{\text{B}0} \exp [-Q/RT_0]}$$

The rate of deactivation was expressed by the equation given in papers [1, 5]

$$\frac{dA_{\text{J}}}{a_{\text{J}}^* dt} = -\frac{d\phi}{dt} = k_{\text{J}} \phi c_{\text{J}} \quad (25)$$

which in the dimensionless form is

$$\frac{dA_{\text{J}}}{d\tau} = -\frac{d\phi}{d\tau} = \phi Y_{\text{J}} \quad (26)$$

The parameters appearing in rate equations (23) and (25) were calculated on

the basis of measurements performed in a rotating basket reactor. The method of measurement and parameter estimation is described in papers [1, 10].

As hydrogen was present in considerable excess owing to which its concentration did not practically vary along the reactor, we assumed $Y_H \approx 1$.

Numerical solution of the model equations

Under quasi-steady state assumption, the reactor model is described by a system of partial differential equations (19—21), two kinetic equations (23) and (26), and boundary conditions (16) and (17). Initial conditions are given by the solution of eqns (19—21) for unit activity. The equations contain only one derivative with respect to time, *i.e.* derivative of activity in the mass balance of catalyst poison which introduces “dynamics” into this system.

Since the temperature does not appear in the rate equation of deactivation (26), the calculation for a given time moment may be divided into two independent steps, *i.e.* calculation of the profile of Y_j and ϕ , and calculation of Y_B and Θ for the calculated profile.

We obtain the first iteration $Y_j^1(Z, \tau + \Delta\tau)$ by transcription of eqn (20) into final differences while we substitute the activity in the time moment τ , *i.e.* $\phi(Z, \tau)$ for activity ϕ . By integrating eqn (26) and rearranging we obtain the following expression

$$\phi(Z, \tau + \Delta\tau) = \phi(Z, \tau) \exp \left[-\Delta\tau \frac{Y_j^1(Z, \tau + \Delta\tau) + Y_j(Z, \tau)}{2} \right] \quad (27)$$

from which we calculate $\phi^1(Z, \tau + \Delta\tau)$. Further iteration $Y_j^{k+1}(Z, \tau + \Delta\tau)$ is to be obtained again from transcription of eqn (20) into final differences, but we must substitute $\phi^k(Z, \tau + \Delta\tau)$ for activity. The calculation is repeated as far as the difference between two successive iterations is smaller than predetermined tolerances

$$\begin{aligned} |\phi^{k+1} - \phi^k| &< \varepsilon_\phi \\ |Y_j^{k+1} - Y_j^k| &< \varepsilon_j, \quad Z \in \langle 0, Z_L \rangle \end{aligned} \quad (28)$$

Eqn (20) was transcribed through virtual profile. The obtained system of linear algebraic equations with tridiagonal matrix was solved by factorization [11].

The mass balance of the key component (19) as well as the enthalpy balance (21) was solved again by iteration. The equations were transcribed into final differences through virtual profile and the reaction rate was written in the form of the Taylor series

$$\dot{\xi}^{k+1}(Z) = \dot{\xi}^k(Z) + \left(\frac{\partial \dot{\xi}^k(Z)}{\partial Y_B} \right)^k (Y_B^{k+1}(Z, \tau + \Delta\tau) - Y_B^k(Z, \tau + \Delta\tau)) +$$

$$+ \left(\frac{\partial \dot{\Theta}(Z)}{\partial \Theta} \right)^k (\Theta^{k+1}(Z, \tau + \Delta\tau) - \Theta^k(Z, \tau + \Delta\tau)) \quad (29)$$

Thus we obtained a system of linear algebraic equations

$$\mathbf{A}X = \mathbf{B} \quad (30)$$

where \mathbf{A} is 5-diagonal matrix of coefficients

$$\begin{aligned} X = & (Y_{\mathbf{B}}^{k+1}(0, \tau + \Delta\tau), \Theta^{k+1}(0, \tau + \Delta\tau), \dots \\ & \dots Y_{\mathbf{B}}^{k+1}(Z_L, \tau + \Delta\tau), \Theta^{k+1}(Z_L, \tau + \Delta\tau)) \end{aligned} \quad (31)$$

and \mathbf{B} is vector of the coefficients of right-hand sides. We solved this system of equations by the method proposed by Němec [12].

The initial conditions were given by solution of the system of model equations for $\phi = 1$ and we took the solution for plug-flow model [1] for the first iteration.

The iterative calculation for a given time step had been employed until the difference between two successive iterations was smaller than predetermined tolerances

$$\begin{aligned} |Y_{\mathbf{B}}^{k+1} - Y_{\mathbf{B}}^k| &< \varepsilon_{\mathbf{B}} \\ |\Theta^{k+1} - \Theta^k| &< \varepsilon_{\Theta} \end{aligned} \quad (32)$$

Results and discussion

The comparison of the numerical results with the described experiment is represented in Figs. 1—5. The following values of dimensionless parameters

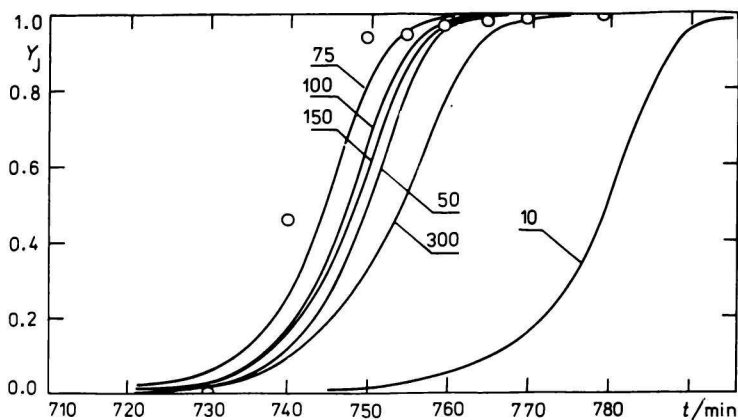


Fig. 1. Time dependence of dimensionless concentration of thiophene at the outlet from reactor for different values of Pe_i (parameter of lines).

correspond to the measurement: $Z_L = 25.67$, $G = 12$, $F = 5.5$, $Pe_h = 0.75$, $\kappa_B = 41.96$, $\alpha_i = 11.43$, $\alpha_K = -7.83$, $\beta = 0.8241$. The values of parameters κ_B , α_i , α_K , and β were determined from the measurements of reaction kinetics in a rotating basket reactor while the values of Z_L and G were calculated from the conditions of measurements. The dimensionless coefficient of heat transfer F was determined from the condition

$$\left(\int_0^{Z_L} \Theta \, dZ \right)_{\text{measured}} \approx \left(\int_0^{Z_L} \Theta \, dZ \right)_{\text{calculated}}$$

and Pe_h was estimated from the maximum temperature when the temperature wave was approximately in the middle of reactor (300 min).

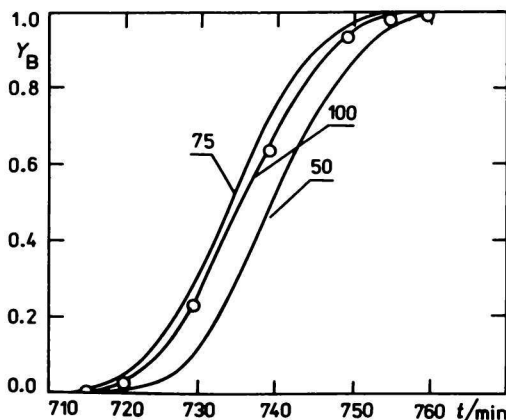


Fig. 2. Time dependence of dimensionless concentration of benzene at the outlet from reactor for $Pe_B = 15$ and a few values of Pe_j (parameter of lines).

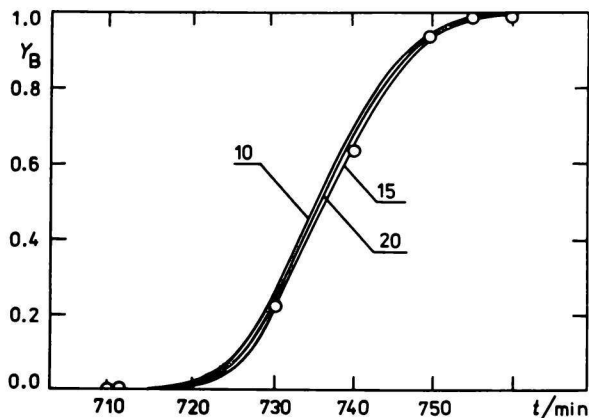


Fig. 3. Time dependence of dimensionless concentration of benzene at the outlet from reactor for a few values of Pe_B (parameter of lines); $Pe_j = 100$.

The time dependence of dimensionless concentrations of thiophene and benzene at the outlet from reactor is represented for different values of Pe_T in Figs. 1 and 2 together with the measured values. While the value $Pe_T = 75$ corresponds best to the measured values of thiophene concentration, the best value for the measured values of benzene concentration is $Pe_T = 100$. Fig. 3 shows the influence of Pe_B on the outlet concentration of benzene. The advance of temperature wave through reactor as well as a comparison with the measured temperature profiles is represented in Fig. 4. Moreover, this figure also contains a comparison with the model of well-mixed regions in series. The dependence of the point of maximum temperature on time is represented in Fig. 5.

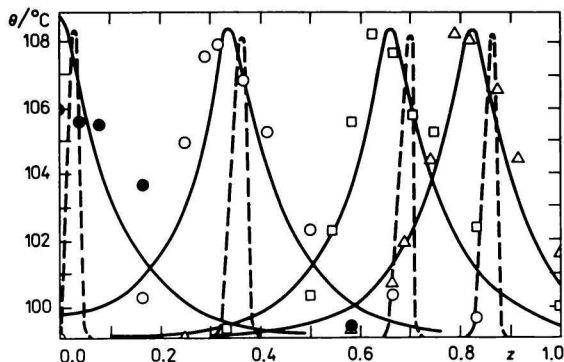


Fig. 4. Advance of temperature wave along reactor for $Pe_B = 15$, $Pe_T = 100$.

— Model with axial dispersion; - - - model of well-mixed regions in series.
Experimental points: ● 0 min; ○ 240 min; □ 480 min; △ 600 min.

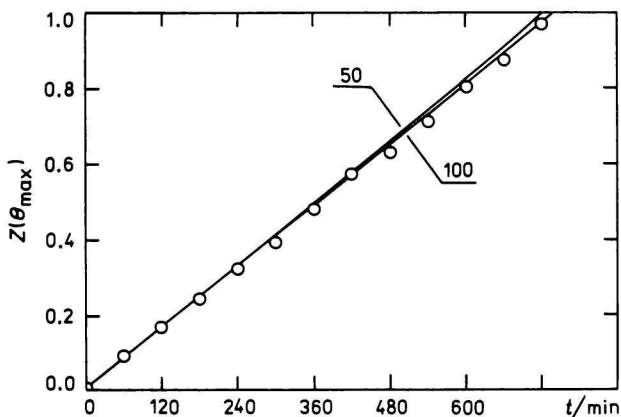


Fig. 5. Dependence of the point of maximum temperature on time for $Pe_B = 15$ and $Pe_T = 50$; 100.

The presented figures show a very good consistence of the model and experiment. While we succeeded in describing the outlet concentrations and maximum temperature in reactor by means of simpler models [1, 2], the model with axial dispersion enables us to express the shape of temperature wave and its advance in reactor as well. Of course, the solution of model equations is more exacting in this case and necessitates a greater consumption of computing time.

Symbols

A_j	dimensionless adsorbed amount of poison	
a_j	adsorbed amount of poison	mol kg ⁻¹
a_j^*	equilibrium adsorbed amount of poison	mol kg ⁻¹
c_B	concentration of key component (benzene)	mol m ⁻³
c_j	concentration of catalyst poison	mol m ⁻³
c_{pg}	specific heat of reaction mixture	J kg ⁻¹ K ⁻¹
D_B, D_j	coefficient of axial dispersion of benzene and catalyst poison, respectively	m ² s ⁻¹
d_i	reactor diameter	m
E	activation energy of catalytic reaction	J mol ⁻¹
F	dimensionless coefficient, eqn (10)	
G	dimensionless coefficient, eqn (10)	
$(-\Delta H)$	molar reaction enthalpy	J mol ⁻¹
h	overall heat transfer coefficient	J m ⁻² s ⁻¹ K ⁻¹
K_∞	adsorption constant for benzene at $T(K)$	Pa ⁻¹
k_∞	frequency factor of catalytic reaction	mol s ⁻¹ kg ⁻¹ Pa ⁻¹
k_j	rate constant of deactivation	m ³ mol ⁻¹ s ⁻¹
L	length of catalytic bed	m
p_B	partial pressure of benzene	Pa
p_H	partial pressure of hydrogen	Pa
Pe_B	Peclet number for benzene, eqn (10)	
Pe_h	Peclet number for heat transfer, eqn (10)	
Pe_j	Peclet number for thiophene, eqn (10)	
Q	adsorption heat of benzene	J mol ⁻¹
R	gas constant	J mol ⁻¹ K ⁻¹
R_S	dimensionless parameter, eqn (10)	
T	temperature	K
ΔT_{ad}	adiabatic increase in temperature,	
	$\Delta T_{ad} = \frac{(-\Delta H)c_{B0}}{Q_g c_{pg}}$	K
t	time	s
t°	characteristic time of deactivation,	
	$t^\circ = \frac{1}{k_j c_{j0}}$	

v	velocity outside layer	m s^{-1}
Y_B	dimensionless concentration of key component (benzene)	
Y_J	dimensionless concentration of catalyst poison	
Y_H	dimensionless concentration of hydrogen	
Z	dimensionless axial coordinate	
z	axial coordinate	m
Z_L	dimensionless length of reactor	
α_i, α_k	dimensionless parameters, eqn (24)	
β	dimensionless parameter, eqn (24)	
δ	dimensionless parameter, eqn (10)	
ε	void fraction	
$\varepsilon_B, \varepsilon_T, \varepsilon_\theta, \varepsilon_\phi$	predetermined tolerances for calculating the profile of benzene, catalyst poison, temperature, and activity	
Θ	dimensionless temperature increase	
κ_B	dimensionless parameter, eqn (24)	
λ_1	coefficient of axial heat conduction	$\text{J K}^{-1} \text{m}^{-1} \text{s}^{-1}$
ν_B	stoichiometric coefficient of key component	
$\bar{\xi}$	dimensionless reaction rate	
ξ_w	reaction rate of catalytic reaction	$\text{mol kg}^{-1} \text{s}^{-1}$
ξ_w^o	reaction rate of catalytic reaction on fresh catalyst corresponding to the composition of reaction mixture and temperature at inlet	$\text{mol kg}^{-1} \text{s}^{-1}$
$\bar{\rho}c_p$	mean heat capacity	$\text{J K}^{-1} \text{m}^{-3}$
ρ_b	bed density	kg m^{-3}
ρ_g	density of gas mixture	kg m^{-3}
τ	dimensionless time	
ϕ	relative activity of catalyst	

Indices

Lower:

Upper:

0 inlet

 k number of iteration

c cooling medium

References

- Ilavský, J., Brunovská, A., Valtýni, J., and Buriánek, J., *Chem. Zvesti* 37, 433 (1983).
- Markoš, J., Brunovská, A., and Ilavský, J., *Chem. Papers*, submitted to publication.
- Hlaváček, V., *Ind. Eng. Chem.* 62, 8 (1970).
- Froment, G. F., *Chemical Reaction Engineering, Advances in Chemistry Series 109*, p. 1. American Chemical Society, Washington, 1972.
- Weng, H. S., Eigenberger, G., and Butt, J. B., *Chem. Eng. Sci.* 30, 1341 (1975).
- Butt, J. B., Weng, H. S., and Eigenberger, G., *Chem.-Ing.-Tech.* 47, 1019 (1975).
- Price, T. H. and Butt, J. B., *Chem. Eng. Sci.* 32, 393 (1977).

8. Do, D. D. and Weiland, R. H., *Chem. Eng. Sci.* 36, 97 (1981).
9. Do, D. D. and Weiland, R. H., *Ind. Eng. Chem. Fundam.* 21, 58 (1982).
10. Markoš, J., Brunovská, A., and Ilavský, J., submitted to publication.
11. Kubíček, M., *Numerické algoritmy řešení chemicko-inženýrských úloh.* (Numerical Algorithms for Solving Chemical Engineering Problems.) Nakladatelství technické literatury (Publishing House of Technical Literature), Alfa Publishers, Prague, Bratislava, 1983.
12. Němec, J., private communication.

Translated by R. Domanský