Numerical solving of coupled systems of parabolic and ordinary differential equations

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Abstract.   Two coupled systems of parabolic and nonlinear ordinary differential equations arising in kinetics of heterogeneous reactions are studied numerically by using computer calculations. Some numerical results are discussed.

Keywords: heterogeneous reactions, adsorption, desorption, parabolic equations.

1   Introduction and formulation of the problem

We study two coupled systems of parabolic and nonlinear ordinary differential equations which describe dynamics of the heterogeneous reactions. In order for the catalytic reaction on a surface to occur, one or more of the reactants must diffuse to the catalyst surface (adsorbent) and adsorb onto it forming one or more intermediates (adsorbates). After conversion (reaction) of the adsorbates the product must desorb and diffuse away from the adsorbent. In the present paper we consider two one-molecular reaction models given in [1]. Both of them include the diffusion of reactant A to the adsorbent K, adsorption of A onto surface of adsorbent K forming adsorbate AK, conversion of AK into a product B, and diffusion of B away from the adsorbent. In one of models, we include a slow desorption of B, while in the other one the desorption of B is assumed to be instantaneous.

Let reactant A and product B of concentrations $a(t, x)$ and $b(t, x)$ occupy domain Ω with surface $\partial\Omega = S_1 \cup S_2$. Here t is time, $x \in \Omega$ is a position, S_2 is a surface of the adsorbent, and $S_1 = \partial\Omega \setminus S_2$. Let the constant s be the surface density of the active sites of S_2 and us be the density of active sites occupied by molecules of adsorbate AK. Here $u \le 1$ is the surface coverage by adsorbed molecules. Then according to Langmuir [2], in the case of instantaneous desorption of B, the adsorption and desorption rates of reactant A and conversion rate of adsorbate AK into product B can be described by the functions $k_f(1 - u)sa|_{S_2}$, $k_r su$, and ksu. Hence, $su' = k_f(1 - u)sa|_{S_2} - k_r su - ksu$, where u' is the partial derivative of u with respect to t. Set $u(0, x) = u_0(x)$. Then

$$u' = k_f(1 - u)a|_{S_2} - (k_r + k)u, \quad u(0, x) = u_0(x). \tag{1}$$

The diffusion of A to S_2 and diffusion of B from S_2 can be described by the systems given in [1],

$$
\begin{cases}
\partial_t a = \kappa_a \Delta a, & t > 0,\ x \in \Omega, \\
\partial_n a|_{S_1} = 0, & t > 0, \\
\kappa_a \partial_n a|_{S_2} = -k_f s(1-u)a|_{S_2} + k_r su, & t > 0, \\
a(0,x) = a_0(x), & x \in \Omega
\end{cases}
\tag{2}
$$

and

$$
\begin{cases}
\partial_t b = \kappa_b \Delta b, & t > 0,\ x \in \Omega, \\
\partial_n b|_{S_1} = 0, & t > 0, \\
\kappa_b \partial_n b|_{S_2} = ksu, & t > 0, \\
b(0,x) = b_0(x), & x \in \Omega.
\end{cases}
\tag{3}
$$

Here κ_a and κ_b are the diffusion coefficients of A and B, Δ is the Laplace operator, and $\partial_n a|_{S_2}$ and $\partial_n b|_{S_2}$ are the outward normal derivatives.

Now we describe the other model given in [1]. Let $u_1 s$ and $u_2 s$ be the densities of the active sites of S_2 occupied by molecules of adsorbate AK and product B, respectively. Obviously, $u_k < 1$, $k = 1, 2$, and $u_1 + u_2 \leq 1$. Then

$$
\begin{cases}
u_1' = k_f(1 - u_1 - u_2)a|_{S_2} - (k_r + k)u_1, & u_1(0,x) = u_{10}(x), \\
u_2' = ku_1 - k_{r1}u_2, & u_2(0,x) = u_{20}(x).
\end{cases}
\tag{4}
$$

Here k_{r1} is a desorption rate constant of B.

Diffusion of A and B can be described by systems

$$
\begin{cases}
\partial_t a = \kappa_a \Delta a, & t > 0,\ x \in \Omega, \\
\partial_n a|_{S_1} = 0, & t > 0, \\
\kappa_a \partial_n a|_{S_2} = -k_f s(1 - u_1 - u_2)a|_{S_2} + k_r su_1, & t > 0, \\
a(0,x) = a_0(x), & x \in \Omega
\end{cases}
\tag{5}
$$

and

$$
\begin{cases}
\partial_t b = \kappa_b \Delta b, & t > 0,\ x \in \Omega, \\
\partial_n b|_{S_1} = 0, & t > 0, \\
\kappa_b \partial_n b|_{S_2} = k_{r1}su_2, & t > 0, \\
b(0,x) = b_0(x), & x \in \Omega.
\end{cases}
\tag{6}
$$

Systems (1)–(3) and (4)–(6) possess the mass conservation laws

$$
\int_\Omega (a + b)\,\mathrm{d}x + \int_{S_2} su\,\mathrm{d}x = \int_\Omega (a_0 + b_0)\,\mathrm{d}x + \int_{S_2} su_0\,\mathrm{d}x,
$$

$$\int\limits_{\Omega} (a + b)\,\mathrm{d}x + \int\limits_{S_2} s(u_1 + u_2)\,\mathrm{d}x = \int\limits_{\Omega} (a_0 + b_0)\,\mathrm{d}x + \int\limits_{S_2} s(u_{10} + u_{20})\,\mathrm{d}x,$$

respectively.

Usually physicists and chemists [3–5] use the steady-state approximation of u which follows from (1),

$$u = \frac{k_f a|_{S_2}}{k_f a|_{S_2} + k_r + k}, \tag{7}$$

and conditions $(2)_3$ and $(3)_3$ written in the form

$$\kappa_a \partial_n a|_{S_2} = -\frac{s k_f k a|_{S_2}}{k_f a|_{S_2} + k_r + k}, \quad \kappa_b \partial_n b|_{S_2} = \frac{s k_f k a|_{S_2}}{k_f a|_{S_2} + k_r + k}.$$

The steady-state approximation of u_1, u_2 and conditions $(5)_3$ and $(6)_3$ can be written in the form

$$u_2 = \frac{k}{k_{r1}} u_1, \quad u_1 = \frac{k_f a|_{S_2}}{k_f (1 + k/k_{r1}) a|_{S_2} + k_r + k},$$

$$\kappa_a \partial_n a|_{S_2} = -k s u_1, \quad \kappa_b \partial_n b|_{S_2} = k s u_1.$$

A lot of papers (see [3–5] and literature there) is devoted to modification of isotherm (7) to more accurately describe the experimental observations. Paper [6] is devoted to study of solvability of system (1)–(3).

The aim of this paper is to study systems (1)–(3) and (4)–(6) numerically by using computer calculations.

This paper is organized as follows. In Section 1, we give the formulation of the problem. In Sections 2 and 3, we give the numerical algorithms and discuss numerical results. Some remarks in Section 4 conclude the paper.

2   Numerical algorithms

Using the dimensionless variables $\bar{t} = t/T$, $\bar{x}_1 = x_1/l$, $\bar{x}_2 = x_2/l$, $\bar{a} = a/a_*$, $\bar{b} = b/a_*$, $\bar{a}_0 = a_0/a_*$, $\bar{b}_0 = b_0/a_*$ and constants $\bar{s} = s/a_* l$, $\bar{k}_f = k_f T a_*$, $\bar{k}_r = k_r T$, $\bar{k}_{r1} = k_{r1} T$, $\bar{k} = kT$, $\bar{\kappa}_a = \kappa_a T/l^2$, $\bar{\kappa}_b = \kappa_b T/l^2$, where T, l, and a_* are the characteristic dimensional units, we rewrite equations (1)–(3) and (4)–(6) in the same form with t, x_1, x_2, a, b, a_0, b_0, k_f, k_r, k_{r1}, k, s, κ_a, and κ_b replaced by $\bar{t}$, $\bar{x}_1$, $\bar{x}_2$, $\bar{a}$, $\bar{b}$, $\bar{a}_0$, $\bar{b}_0$, $\bar{k}_f$, $\bar{k}_r$, $\bar{k}_{r1}$, $\bar{k}$, $\bar{s}$, $\bar{\kappa}_a$, and $\bar{\kappa}_b$. For simplicity in what follows, we omit the bar and treat equations (1)–(3) and (4)–(6) as dimensionless.

To get the numerical solution of systems (1)–(3) and (4)–(6) we use the finite-difference schemes and consider two-dimensional domain $\Omega = [0,1] \times [0,1]$ with $S_2 = \{(x_1, x_2): x_1 \in [0,1], x_2 = 0\}$.

Assume that

$$t_k = k\tau, \quad t_{k+1/2} = \left(k + \frac{1}{2}\right)\tau, \quad 0 \le k \le M, \quad \tau = \frac{\widetilde{T}}{M},$$

$$x_{1i} = ih_1, \quad 0 \le i \le N_1, \ h_1 = \frac{1}{N_1}; \quad x_{2j} = jh_2, \quad 0 \le j \le N_2, \ h_2 = \frac{1}{N_2}.$$

Set $a_{ij}^k = a(t_k, x_{1i}, x_{2j}), b_{ij}^k = b(t_k, x_{1i}, x_{2j}), u_{1i}^k = u_1(t_k, x_{1i}), u_{2i}^k = u_2(t_k, x_{1i})$ and $a_{ij}^{k+1/2} = a(t_{k+1/2}, x_{1i}, x_{2j}), b_{ij}^{k+1/2} = b(t_{k+1/2}, x_{1i}, x_{2j})$.

Let the difference operators Λ_1 and Λ_2 be defined by $\Lambda_1 v_{ij} = (v_{i-1,j} - 2v_{ij} + v_{i+1,j})/h_1^2, \Lambda_2 v_{ij} = (v_{i,j-1} - 2v_{ij} + v_{i,j+1})/h_2^2$ and let I be the identity operator.

To approximate the differential problems (1)–(3) and (4)–(6) the alternating directions implicit method [7] is used. We write the following difference scheme to problem (5):

$$\left(I - \frac{\tau\kappa_a}{2}\Lambda_1\right)a_{ij}^{k+1/2} = \left(I + \frac{\tau\kappa_a}{2}\Lambda_2\right)a_{ij}^k, \tag{8}$$

$$i = 1, 2, \ldots, N_1 - 1; \ j = 1, 2, \ldots, N_2 - 1,$$

$$a_{0j}^{k+1/2} = a_{1j}^{k+1/2}, \quad a_{N_1j}^{k+1/2} = a_{N_1-1,j}^{k+1/2}, \quad j = 1, 2, \ldots, N_2 - 1, \tag{9}$$

$$\left(I - \frac{\tau\kappa_a}{2}\Lambda_2\right)a_{ij}^{k+1} = \left(I + \frac{\tau\kappa_a}{2}\Lambda_1\right)a_{ij}^{k+1/2}, \tag{10}$$

$$i = 1, 2, \ldots, N_1 - 1; \ j = 1, 2, \ldots, N_2 - 1,$$

$$a_{i0}^{k+1} = \frac{\kappa_a}{\kappa_a + h_2 s k_f(1 - u_{1,i}^k - u_{2,i}^k)}a_{i1}^{k+1} + \frac{h_2 s k_r u_{1,i}^k}{\kappa_a + h_2 s k_f(1 - u_{1,i}^k - u_{2,i}^k)}, \tag{11}$$

$$i = 1, 2, \ldots, N_1 - 1,$$

$$a_{iN_2}^{k+1} = a_{i,N_2-1}^{k+1}, \quad i = 1, 2, \ldots, N_1 - 1, \tag{12}$$

$$a_{0j}^{k+1} = a_{1j}^{k+1}, \quad a_{N_1j}^{k+1} = a_{N_1-1,j}^{k+1}, \quad j = 1, 2, \ldots, N_2 - 1, \tag{13}$$

for all $k = 0, 1, \ldots, M - 1$, with the discrete initial condition

$$a_{ij}^0 = a_{0,ij}, \quad i = 1, 2, \ldots, N_1 - 1; \ j = 1, 2, \ldots, N_2 - 1. \tag{14}$$

The sweeping method [7] is used for solving problem (8), (9) for fixed k and j, and (10)–(12) for fixed k and i.

To write the difference scheme to problem (6) we have to replace function a by b, the parameter κ_a by κ_b in equations (8)–(14) and use the following boundary condition for function b at $x_2 = 0$ instead of approximation (11):

$$b_{i0}^{k+1} = b_{i1}^{k+1} + \frac{h_2 s k_{r1}}{\kappa_b}u_{2,i}^k, \quad i = 1, 2, \ldots, N_1 - 1. \tag{15}$$

The values of u_1 and u_2 at each time step are calculated explicitly by the scheme

$$u_{1,i}^{k+1} = u_{1,i}^k + 0.5\tau\Big\{\big[k_f(1 - u_{1,i}^k - u_{2,i}^k)a_{i0}^{k+1} - (k_r + k)u_{1,i}^k\big]$$
$$+ \big[k_f(1 - u_{1,i}^{k-1} - u_{2,i}^{k-1})a_{i0}^k - (k_r + k)u_{1,i}^{k-1}\big]\Big\}, \tag{16}$$
$$u_{2,i}^{k+1} = u_{2,i}^k + 0.5\tau\big[\big(ku_{1,i}^k - k_{r1}u_{2,i}^k\big) + \big(ku_{1,i}^{k-1} - k_{r1}u_{2,i}^{k-1}\big)\big]$$

for $k = 1, \ldots, M - 1$ and

$$u_{1,i}^1 = u_{1,i}^0 + 0.5\tau\big[k_f\big(1 - u_{1,i}^0 - u_{2,i}^0\big)a_{i0}^1 - (k_r + k)u_{1,i}^0\big], \quad u_{1,i}^0 = u_{10,i},$$
$$u_{2,i}^1 = u_{2,i}^0 + 0.5\tau\big(ku_{1,i}^0 - k_{r1}u_{2,i}^0\big), \quad u_{2,i}^0 = u_{20,i} \tag{17}$$

for each $i = 1, 2, \ldots, N_1 - 1$.

For problem (1) we use the approximation

$$u_i^{k+1} = u_i^k + 0.5\tau\big\{\big[k_f\big(1 - u_i^k\big)a_{i0}^{k+1} - (k_r + k)u_i^k\big]$$
$$+ \big[k_f\big(1 - u_i^{k-1}\big)a_{i0}^k - (k_r + k)u_i^{k-1}\big]\big\} \tag{18}$$

for $k = 1, \ldots, M - 1$ and

$$u_i^1 = u_i^0 + 0.5\tau\big[k_f\big(1 - u_i^0\big)a_{i0}^1 - (k_r + k)u_i^0\big], \quad u_i^0 = u_{0,i} \tag{19}$$

for each $i = 1, 2, \ldots, N_1 - 1$. The boundary conditions at $x_2 = 0$ (11) and (15) are written as follows:

$$a_{i0}^{k+1} = \frac{\kappa_a}{\kappa_a + h_2 sk_f(1 - u_i^k)}a_{i1}^{k+1} + \frac{h_2 sk_r u_i^k}{\kappa_a + h_2 sk_f(1 - u_i^k)}, \tag{20}$$

$$b_{i0}^{k+1} = b_{i1}^{k+1} + \frac{h_2 skr}{\kappa_b}u_i^k. \tag{21}$$

The local approximation error for inner points of $(0, T) \times \Omega$ is $O(\tau^2 + h_1^2 + h_1^2)$ [7]. The boundary conditions are changed with the accuracy $O(h_1)$ at $x_1 = 0$, $x_1 = 1$ and $O(h_2)$ at $x_2 = 0$, $x_2 = 1$. The approximation of (1) and (4) is of the first order with respect to time variable.

In the case $\partial_{x_2} a_0(x)|_{x_2=0;1} = \partial_{x_2} b_0(x)|_{x_2=0;1} = 0$ the difference solutions satisfy the discrete analogues of the mass conservation laws:

$$h_1 h_2 \sum_{i=1}^{N_1-1} \sum_{j=1}^{N_2-1} \big(a_{ij}^{k+1} + b_{ij}^{k+1}\big) + sh_1 \sum_{i=1}^{N_1-1} u_i^{k+1}$$
$$= h_1 h_2 \sum_{i=1}^{N_1-1} \sum_{j=1}^{N_2-1} \big(a_{ij}^k + b_{ij}^k\big) + sh_1 \sum_{i=1}^{N_1-1} u_i^k, \tag{22}$$

$$h_1 h_2 \sum_{i=1}^{N_1-1} \sum_{j=1}^{N_2-1} \big(a_{ij}^{k+1} + b_{ij}^{k+1}\big) + sh_1 \sum_{i=1}^{N_1-1} \big(u_{1,i}^{k+1} + u_{2,i}^{k+1}\big)$$
$$= h_1 h_2 \sum_{i=1}^{N_1-1} \sum_{j=1}^{N_2-1} \big(a_{ij}^k + b_{ij}^k\big) + sh_1 \sum_{i=1}^{N_1-1} \big(u_{1,i}^k + u_{2,i}^k\big). \tag{23}$$

The numerical experiments for different values of h_1, h_2 and τ show the stable behavior of the numerical solution. We also solved problem (1)–(4) by using the implicit difference scheme. Calculations show that this scheme is stable for $\tau \leq 0.25h^2/\kappa$, $h = \min\{h_1, h_2\}$, $\kappa = \max\{\kappa_a, \kappa_b\}$. The difference between results of explicit and implicit schemes is small.

From the physical point of view $a(t,x) \to 0$, $u(t,x_1) \to 0$, $b(t,x) \to \int_\Omega a_0(x)\,dx$ as $t \to \infty$ in the case of instantaneous adsorption and $a(t,x) \to 0$, $u_1(t,x_1) \to 0$, $u_2(t,x_1) \to 0$, $b(t,x) \to \int_\Omega a_0(x)\,dx$ as $t \to \infty$ for the slow adsorption. Calculations show that numerical solutions possess this property.

3 Numerical results

Results are illustrated in Figs. 1–6 for $\overline{\Omega} = [0,1] \times [0,1]$, $S_2 = \{(x_1, x_2)\colon x_1 \in [0,1], x_2 = 0\}$, $\kappa_a = \kappa_b = 0.1$, $s = 10$, $u_0 = u_{10} = u_{20} = b_0 = 0$,

$$a_0 = 20\big(\exp(-2x_1) - \exp(-2)\big)/\big(1 - \exp(-2)\big).$$

The results presented in this section are computed with $\tau = h_1 = h_2 = 0.01$.

Usually surfaces are not homogeneous and constant k_f, k_r, k, and k_{r1} depend on many factors including processing of surfaces. Therefore experimental observations of their values may be different. Values of constants that we use are given in captions.

Fig. 1 demonstrates the behavior of functions $a(t,0,x_2)$ from models (1)–(3) and (4)–(6) versus x_2 for five values of t and $k_f = 0.2$, $k_r = 1$, $k_{r1} = 0.1$, $k = 0.1$. The figure shows a difference between curves for $t > 1$ which for large t tends to zero. Calculations also shows that for large k_{r1} ($k_{r1} \geq 1$) this difference practically is zero and it increases as $k_{r1} < 1$ decreases. For large k_f ($k_f \geq 1$), this difference also is small.
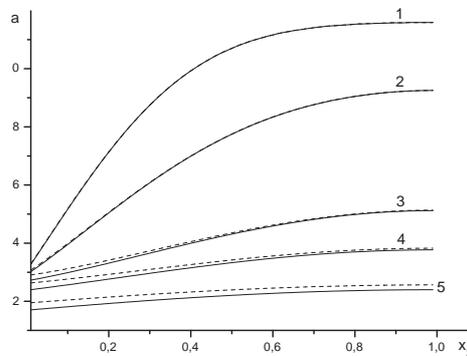

Fig. 1. Graphs of function $a(t,0,x_2)$ from systems (1)–(3) (solid line) and (4)–(6) (dash) for $k_f = 0.2$, $k_r = 1$, $k_{r1} = 0.1$, $k = 0.1$: 0.5 – curves 1, 1 – curves 2, 3 – curves 3, 5 – curves 4, 10 – curves 5.

Figs. 2(a) and 2(b) illustrate the behavior of $b(t,0,x_2)$ from models (1)–(3) and (4)–(6) versus x_2 for five values of t and $k_f = 0.2$, $k_r = 1$, $k_{r1} = 1$, $k = 0.1$ (Fig. 2(a)) and $k_f = 0.2$, $k_r = 1$, $k_{r1} = 0.1$, $k = 0.1$ (Fig. 2(b)). We observe a decrease of the difference between curves as k_{r1} increases.

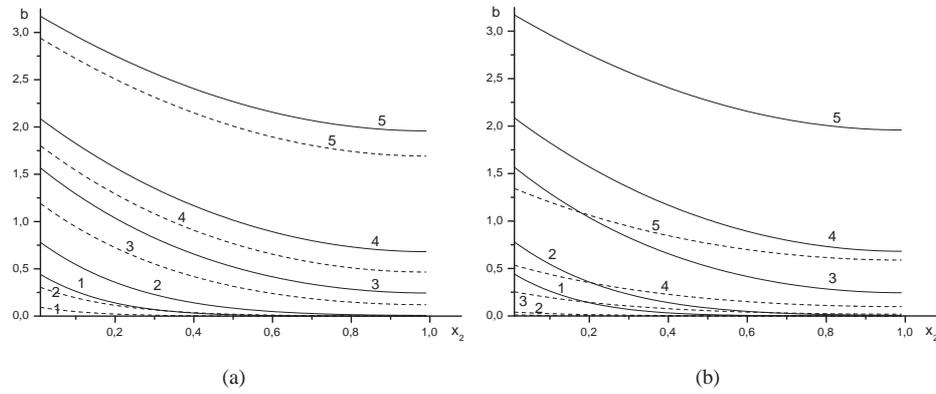(a)   (b)

Fig. 2. Graphs of function $b(t, 0, x_2)$ from systems (1)–(3) (solid line) and (4)–(6)
(dash) for $k_f = 0.2$, $k_r = 1$, $k = 0.1$, (a) $k_{r1} = 1$, (b) $k_{r1} = 0.1$: 0.5 – curves 1,
1 – curves 2, 3 – curves 3, 5 – curves 4, 10 – curves 5.

In Fig. 3 we exhibit the graph of function $b(t, 0, x_2)$ from system (1)–(3) for
$k_f = 1$, $k_r = 0.1$, $k = 1$. The graph shows that $b(t, 0, x_2)$ possesses maximum values for
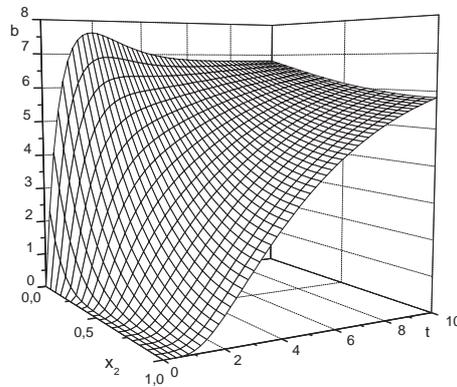small x_2.

Fig. 3. Graph of function $b(t, 0, x_2)$ from system (1)–(3) for $k_f = 1$, $k_r = 0.1$, $k = 1$.

In Fig. 4 we exhibit the behavior of $a(t, 0, x_2)$ from model (4)–(6) for five values
of t and $k_r = 0.1$, $k_{r1} = 1$, $k = 1$, and $k_f = 0.2$ (solid line), $k_f = 1$ (dash line).
For small t, the difference increases as x_2 decreases (see curves 1 and 2). Curves 3 and
4 demonstrate a difference practically independent of x_2. For large t (see curves 5) this
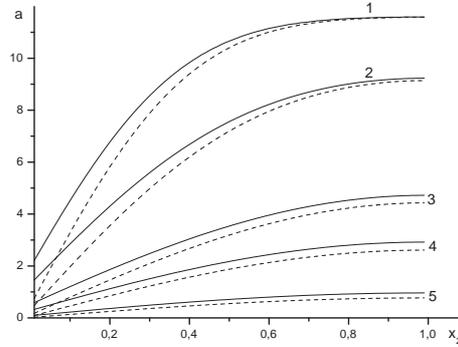difference increases as x_2 grows.

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Fig. 4. Graphs of function $a(t, 0, x_2)$ from system (4)–(6) for $k_r = 0.1$, $k_{r1} = 1$, $k = 1$, $k_f = 0.2$ (solid line) and $k_f = 1$ (dash), and t: 0.5 – curves 1, 1 – curves 2, 3 – curves 3, 5 – curves 4, 10 – curves 5.

Figs. 5(a) and 5(b) exhibit the behavior of $u(t, x_1)$ (bullets) from model (1)–(3) and $u_1(t, x_1)$ (solid line) and $u_2(t, x_1)$ (dash line) from model (4)–(6) for $k_f = 0.2$, $k_r = 1$, $k_{r1} = 0.1$, $k = 1$ (Fig. 5(a)) and $k_f = 0.2$, $k_r = 0.01$, $k_{r1} = 1$, $k = 1$ (Fig. 5(b)). Figures show, that difference between functions $u(t, x_1)$ and $u_1(t, x_1)$ is small for $k_{r1} \in [0.1; 1]$. The dependance of $u_2(t, x_1)$ on k_{r1} is strong, and $u_2(t, x_1)$ grows as k_{r1} decreases. We also see, that $u_1(t, x_1)$, $u_2(t, x_1)$, and $u(t, x_1)$ possess maximal values at moments $t_1(x_1)$ and $t_2(x_1)$, respectively, depending on x_1. Calculations also show that $t_2(x_1) > t_2(x_1)$.
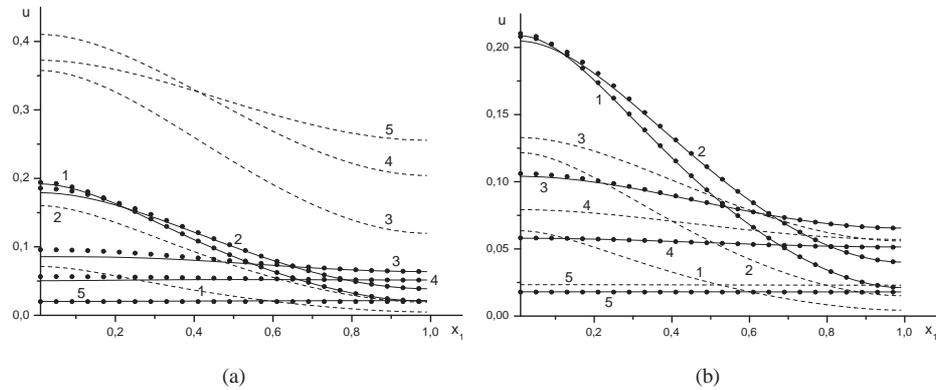

(a)   (b)

Fig. 5. Graphs of functions $u(t, 0, x_1)$ (bullets) from system (1)–(3) and $u_1(t, 0, x_1)$ (solid line), $u_2(t, 0, x_1)$ (dash) from system (4)–(6) for $k_f = 0.2$, $k_{r1} = 0.1$, $k = 1$, (a) $k_r = 1$, (b) $k_r = 0.01$, and t: $0.5 - 1$, $1 - 2$, $3 - 3$, $5 - 4$, $10 - 5$.

Figs. 6(a) and 6(b) demonstrate graphs of $u_1(t, x_1)$ and $u_2(t, x_1)$, respectively. Times $t_1(x_1)$ and $t_2(x_1)$ of maximal values of u_1 and u_2 depend on data k_f, k_r, k_{r1},

k, κ_a, κ_b, and s. If difference $t_2(x_1) - t_1(x_1)$ is small, then u_2 influences the behavior of a more significantly. In the other cases this influence is small. Because of the boundary condition $(6)_3$ the dependance of $b(t, 0, x_2)$ on $u_2(t, x_1)$ is very strong.
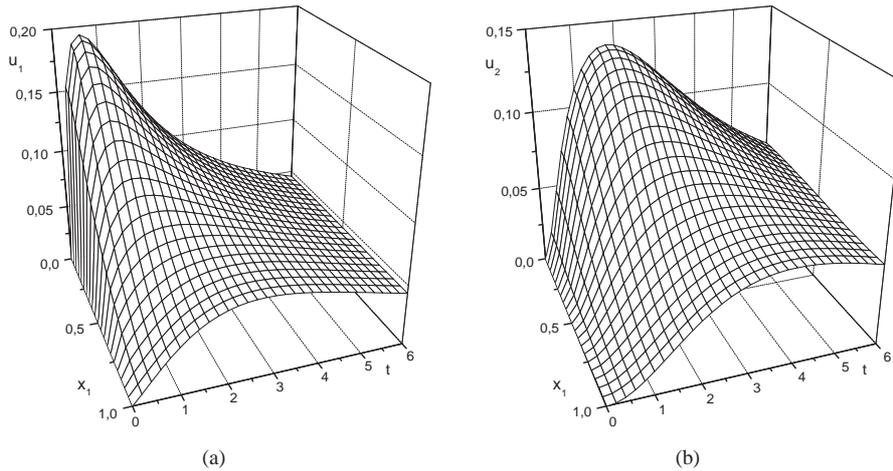

(a) (b)

Fig. 6. Graph of functions (a) $u_1(t, x_1)$, (b) $u_2(t, x_1)$ from system (4)–(6) for $k_f = 0.2$, $k_r = 1$, $k_{r1} = 1$, $k = 1$.

4 Concluding remarks

We examined numerically two models of unimolecular heterogeneous reactions. In one model, desorption of the product is instantaneous while in the other one the desorption rate of the product is bounded. Boundary conditions of model (1)–(3) demonstrate the qualitative behavior of its solutions:

- the increase of k_f decreases a, but increases b,
- the increase of k_r increases a, but decreases b,
- the increase of k decreases a, but increases b.

  Boundary conditions of model (4)–(6) show that:

- the increase (decrease) of k_{r1} decreases (increases) the difference of models (1)–(3) and (4)–(6),
- the increase of k increases b,
- the increase of k_r decreases u_2 and, hence, it decreases b.

  Numerical calculations show that in general functions a defined by models (1)–(3) and (4)–(6) differs a little, but the difference of b is significant.

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