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NONLINEAR MODEL OF THE THREE-COMPONENTS COMPETITIVE ADSORPTION USING LANGMUIR EQUILIBRIUM

A basis for the mathematical modeling of non-isothermal gas competitive adsorption in a porous solid using Langmuir equilibrium is given. High-performance analytical solutions of considered adsorption models based on the Heaviside operating method and Landau's decomposition and linearization approach of Langmuir equilibrium by expanding into a convergent series in the temperature phase transition point are proposed.

Numerical experiments results based on high-speed computations on multicore computers are presented.

Key words and phrases: competitive adsorption, nanoporous medium, diffusion coefficient, competitive Langmuir equilibrium, Heaviside operating method, high-performance calculations.

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Introduction

The experimental and theoretical study of the competitive adsorption and diffusion of several gases through a nanoporous solid and the instantaneous (out of equilibrium) distribution of the adsorbed phases is particularly important in many fields, such as gas separation, heterogeneous catalysis, purification of confined atmospheres, reduction of exhaust emissions contributing to global warming, etc.[1]. Taking into account the influence of physical factors that limit the adsorption kinetics on the surface of nanopores, the quality of the mathematical models for the adsorption of exhaust gases (hydrocarbon components, CO_2) in a microporous bed determines the effectiveness of technological solutions for the neutralization of gas emissions [2, 3, 4, 5, 6, 7, 8].

However, most of these models do not fully reflect the complex spatial-temporal representations of the course of all components of complex mass transfer in the intercrystallite space and in the intracrystallite space, including the internal kinetics of the phase transition taking into account the geometric characteristics of transfer areas [6, 7].

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In the proposed paper, which is a development of papers [8, 9, 10, 11], substantiated and developed highly productive methods for mathematical modeling of three-component adsorption in the microporous solid based on a system of spatiotemporal equations of heat and mass transfer in partial derivatives and generalized Langmuir equation. For modeling, we use the high-performance methods of the Heaviside operational calculus and the decomposition approach for expansion the adsorption equilibrium.

1 COMPETITIVE N-COMPONENT ADSORPTION MODEL IN GENERAL FORMULATION

The presented model is analogous to the biporous model [2, 3, 5, 6]. Developing the approach described by Rhutwen and Karger [7, 8] and Petryk et al. [9] concerning the construction of a complex process of competitive adsorption and diffusion, one should dwell on the most important defining hypotheses limiting the process.

The general hypothesis adopted in developing the presented model in the most general formulation concludes that the competitive n-component adsorption interaction between adsorption molecules of several gases (two or more) and active adsorption centers on the phase separation surfaces in the nanoporous crystallites is determined on the basis of the nonlinear competitive equilibrium function of the Langmuir type, taking into account the physical assumptions [7]:

1. Competitive adsorption is caused by the dispersion forces whose interaction is established by Lennard-Jones and the electrostatic forces of gravity and repulsion, the mechanism of which is described by Van der Waals [8]. The competitive diffusion process involves two types of mass transfer: diffusion in the macropores (intercrystallite space) and diffusion in the micropores of crystallites (intracrystallite space).

2. During the evolution of the system towards equilibrium there is a concentration gradient in the macropores and in the micropores.

3. Competitive adsorption and diffusion occurs in active adsorbent centers, distributed throughout the inner surface of the nanoporous[7, 8]. All crystallites are spherical and have the same radius R, the crystallite bed is uniformly packed.

Taking into account the above, we have developed a nonlinear competitive adsorption model in the form of these hypotheses:

$$\frac{\partial C_j\left(t,Z\right)}{\partial t} = \frac{D_{inter_j}}{l^2}\frac{\partial^2 C_j}{\partial Z^2} - e_{inter_j}\frac{D_{intra_j}}{R^2}\left(\frac{\partial Q_j}{\partial X}\right)_{X=1}, \tag{1}$$

$$\frac{\partial Q_j\left(t,X,Z\right)}{\partial t} = \frac{D_{intra_j}}{R^2}\left(\frac{\partial^2 Q_j}{\partial X^2} + \frac{2}{X}\frac{\partial Q_j}{\partial X}\right) \tag{2}$$

with initial conditions:

$$C_j\left(t,Z\right)_{|t=0} = 0,\ \ Q_j\left(t,X,Z\right)_{|t=0} = 0,\ \ X \in (0,1)\,,\ \ j = \overline{1,3} \tag{3}$$

and boundary conditions for coordinate X of the crystallite (particle):

$$\frac{\partial}{\partial X}Q_j\left(t,X,Z\right)_{|X=0} = 0. \tag{4}$$

In expressions (1),(2) the function

$$Q_j\left(t, X=1, Z\right)_{|X=1} = K_j C_j\left(t, Z\right) \left[1 + K_1 C_1\left(t, Z\right) + K_2 C_2\left(t, Z\right) + K_3 C_3\left(t, Z\right)\right]^{-1} \qquad (5)$$

is the Langmuir competitive adsorption equilibria with boundary conditions on coordinate Z:

$$C_j\left(t, Z\right)_{|Z=1} = C_j^{in}, \ \frac{\partial}{\partial Z} C_j\left(t, Z\right)_{|Z=0} = 0. \qquad (6)$$

Here $c_j, q_j, j = \overline{1,3}$ is the current concentrations of the diffusion adsorbent components in the gas phase and micropores of the adsorbent particles, $c_{\infty j}, q_{\infty j}$ is the corresponding equilibrium concentrations of the adsorbent components in the gas and adsorbed phase, $\tilde{\mathrm{K}}_j = \mathrm{q}_{\infty_j}/\mathrm{c}_{\infty_j}$ is the adsorption constant of the j-th component of the adsorbent, $\mathrm{K}_j = 1/\tilde{\mathrm{K}}_j, j = \overline{1,3}$, $\varepsilon_{\text{inter}}$ is the macroporosity of the media,

$$\mathrm{e}_{\text{inter}_j} = \frac{\varepsilon_{\text{inter}} c_j}{\varepsilon_{\text{inter}} c_j + \left(1 - \varepsilon_{\text{inter}}\right) q_j} \approx \frac{\varepsilon_{\text{inter}}}{\left(1 - \varepsilon_{\text{inter}}\right) \tilde{\mathrm{K}}_j}.$$

Next, we perform the decomposition of nonlinear system (1)-(5). The nonlinear function of the competitive Langmuir adsorption equilibrium is as follows [10]:

$$\varphi_j\left(C_1, C_2, C_3\right) = \frac{C_j\left(t, Z\right)}{1 + K_1 C_1\left(t, Z\right) + K_2 C_2\left(t, Z\right) + K_3 C_3\left(t, Z\right)}, j = \overline{1,3}. \qquad (7)$$

We decompose diffusion components of the adsorbate [13] into a Maclaurin series at the point of zero concentrations:

$$\begin{aligned} \varphi_j^0\left(C_1, C_2, C_2\right) = \varphi_j^0 + \left(\frac{\partial^2 \varphi_j^0}{\partial C_1 \partial C_2} C_1 C_2 + \frac{\partial^2 \varphi_j^0}{\partial C_1 \partial C_3} C_1 C_3 + \frac{\partial^2 \varphi_j^0}{\partial C_2 \partial C_3} C_2 C_3\right) + \\ + \left(\frac{\partial \varphi_j^0}{\partial C_1} C_1 + \frac{\partial \varphi_j^0}{\partial C_2} C_2 + \frac{\partial \varphi_j^0}{\partial C_3} C_3\right) + \frac{1}{2}\left(\frac{\partial^2 \varphi_j^0}{\partial C_1^2} C_1^2 + \frac{\partial^2 \varphi_j^0}{\partial C_2^2} C_2^2 + \frac{\partial^2 \varphi_j^0}{\partial C_3^2} C_3^2\right) + \ldots \end{aligned} \qquad (8)$$

where $\varphi_j^0 = \varphi_j\left(0, 0, 0\right), j = \overline{1,3}$. As a result, we obtain the following decompositions for (5) of the second order of accuracy:

$$\begin{aligned} Q_1\left(t, X=1, Z\right)_{|X=1} &= K_1\left(C_1 - K_1 C_1^2 - K_2 C_1 C_2 - K_3 C_1 C_3\right), \\ Q_2\left(t, X=1, Z\right)_{|X=1} &= K_2\left(C_2 - K_2 C_2^2 - K_1 C_1 C_2 - K_3 C_2 C_3\right), \\ Q_3\left(t, X=1, Z\right)_{|X=1} &= K_3\left(C_3 - K_3 C_3^2 - K_1 C_1 C_3 - K_2 C_2 C_3\right). \end{aligned} \qquad (9)$$

Assuming that $K_1 = \max\left\{K_j, K_j < 1\right\}_{j=1}^{3}$ where $\varepsilon = K_1^2 << 1$ (small parameter), problem (1)-(6), taking into account the approximated kinetic equations of phase transformation (9) containing a small parameter ε, is a boundary problem for a nonlinear system of partial differential equations. The solution of problem (1)-(5) will be sought with the help of asymptotic expansions in the small parameter ε in the form of the following series [13]:

$$C_j\left(t, Z\right) = C_{j_0}\left(t, Z\right) + \varepsilon C_{j_1}\left(t, Z\right) + \varepsilon^2 C_{j_2}\left(t, Z\right) + \ldots, \qquad (10)$$

$$Q_j\left(t, X, Z\right) = Q_{j_0}\left(t, X, Z\right) + \varepsilon Q_{j_1}\left(t, X, Z\right) + \varepsilon^2 Q_{j_2}\left(t, X, Z\right) + \ldots, j = \overline{1,3}. \qquad (11)$$

As the result of substituting the asymptotic sum (10), (11) into equations (1)-(6) and replacing variables $N_{j_m} = X \cdot Q_{j_m}$, the initial nonlinear boundary problem (1)-(6) is parallelized into two types of linearized boundary problems.

Problem $A_{j_0}, j = \overline{1,3}$: to find a solution of partial differential equations system for the area $D = \{(t, X, Z) : t > 0,\ X \in (0,1), Z \in (0,1)\}$.

$$\frac{\partial}{\partial t} C_{j_0}(t, Z) = \frac{D_{inter_j}}{l^2} \frac{\partial^2 C_{j_0}}{\partial Z^2} - e_{inter_j} \frac{D_{intra_j}}{R^2} \left(\frac{\partial N_{j_0}}{\partial X} - N_{j_0} \right)_{X=1}, \tag{12}$$

$$\frac{\partial}{\partial t} N_{j_0}(t, X, Z) = \frac{D_{intra_j}}{R^2} \frac{\partial^2 N_{j_0}}{\partial X^2} \tag{13}$$

with initial conditions:

$$C_{j_0}(t, Z)_{|t=0} = 0;\ N_{j_0}(t, X, Z)_{|t=0} = 0;\ X \in (0,1),\ j = \overline{1,3} \tag{14}$$

and boundary conditions for coordinate X of the crystallite:

$$N_{j_0}(t, X, Z)_{|X=0} = 0;\ N_{j_0}(t, X, Z)_{|X=1} = K_j C_{j_0}(t, Z), j = \overline{1,3} \tag{15}$$

The boundary conditions for coordinate Z are as follows:

$$C_{j_0}(t, Z)_{|Z=1} = 1;\ \frac{\partial}{\partial Z} C_{j_0}(t, Z)_{|Z=0} = 0. \tag{16}$$

Problem $A_m, m = \overline{1,\infty}$: to find in the area D a limited solution for the system of equations:

$$\frac{\partial C_{j_m}}{\partial t}(t, Z) = \frac{D_{inter_j}}{l^2} \frac{\partial^2 C_{j_m}}{\partial Z^2} - e_{\mathrm{inter}_j} \frac{D_{intra_j}}{R^2} \left(\frac{\partial N_{j_m}}{\partial X} - N_{j_m} \right)_{X=1}, \tag{17}$$

$$\frac{\partial}{\partial t} N_{j_m}(t, X, Z) = \frac{D_{intra_j}}{R^2} \frac{\partial^2 N_{j_m}}{\partial X^2} \tag{18}$$

with zero initial conditions:

$$C_{j_m}(t, Z)_{|t=0} = 0;\ N_{j_m}(t, X, Z)_{|t=0} = 0,\ j = \overline{1,3} \tag{19}$$

boundary conditions for coordinate X of the crystallite:

$$N_{j_m}(t, X, Z)_{|X=0} = 0;\ N_{j_m}(t, X, Z)_{X=1} = K_j C_{j_m}(t, Z) - F_{j_m}(t, Z), j = \overline{1,3}, \tag{20}$$

$$F_{j_m}(t, Z) = \sum_{s=0}^{m-1} \sum_{k=1}^{3} \frac{K_j K_k}{K_1^2} C_{j_s}(t, Z)\, C_{k_{m-1-s}}(t, Z), j = \overline{1,3}. \tag{21}$$

The boundary conditions for coordinate Z are as follows:

$$C_{j_m}(t, Z)_{|Z=1} = 0;\ \frac{\partial}{\partial Z} C_{j_m}(t, Z)_{|Z=0} = 0. \tag{22}$$

The construction methodology of an analytical solution. The Heaviside operating method [13] is used to find solutions C_{j_m} and Q_{j_m} of linearized system of problems (1)-(6).

Assuming that the required functions C_{j_m} and Q_{j_m} ($N_{>m} = X \cdot Q_{j_m}$) are Laplace originals, in Laplace images we obtain the next problems.

Problem A_0^*:

$$\frac{\partial^2 C_{j0}^*}{\partial Z^2} = \frac{l^2}{\mathrm{D}_{\mathrm{inter}_j}} pC_{j0}^* + \frac{3}{e_{\mathrm{inter}_j}} \frac{l^2}{\mathrm{R}^2} \frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{D}_{\mathrm{inter}_j}} \left(\frac{\partial N_{j0}^*}{\partial X} - N_{j0}^* \right)_{X=1}, \tag{23}$$

$$\frac{\partial^2 N_{j0}^*}{\partial X^2} - \frac{\mathrm{R}^2}{\mathrm{D}_{\mathrm{intra}_j}} p\, N_{j0}^* = 0 \tag{24}$$

with boundary conditions for coordinate X of the crystallite:

$$N_{j0}^* \left(p, X, Z\right)_{|X=0} = 0; \; N_{j0}^* \left(p, X, Z\right)_{|X=1} = K_j C_{j0}^* \left(p, Z\right), j = \overline{1,3}. \tag{25}$$

The boundary conditions for coordinate Z are as follows:

$$C_{j0}^* \left(p, Z\right)_{|Z=1} = C_j^{in}/p, \; \frac{\partial}{\partial Z} C_{j0}^* \left(p, Z\right)_{|Z=0} = 0. \tag{26}$$

Problem $A_m^*, m = \overline{1, \infty}$:

$$\frac{\partial^2 C_{jm}^*}{\partial Z^2} = \frac{l^2}{\mathrm{D}_{\mathrm{inter}_j}} pC_{jm}^* + \frac{3}{e_{\mathrm{inter}_j}} \frac{l^2}{\mathrm{R}^2} \frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{D}_{\mathrm{inter}_j}} \left(\frac{\partial N_{jm}^*}{\partial X} - N_{jm}^* \right)_{X=1}, \tag{27}$$

$$\frac{\partial^2 N_{jm}^*}{\partial X^2} - \frac{\mathrm{R}^2}{\mathrm{D}_{\mathrm{intra}_j}} p\, N_{jm}^* = 0. \tag{28}$$

The boundary conditions for coordinates X and Z are as follows:

$$N_{jm}^* \left(p, X, Z\right)_{|X=0} = 0; \; N_{im}^* \left(p, X, Z\right)_{|X=1} = K_j C_{jm}^* \left(p, Z\right) - F_{jm}^* \left(p, Z\right), j = \overline{1,3}, \tag{29}$$

$$C_{jm}^* \left(p, Z\right)_{|Z=1} = 0; \; \frac{\partial}{\partial Z} {}_{jm}^* \left(p, Z\right)_{|Z=0} = 0. \tag{30}$$

Here $C_{jm}^* \left(p, Z\right) = \int_0^\infty C_{jm} \left(t, Z\right) e^{-pt} dt$, $N_{jm}^* \left(p, X, Z\right) = \int_0^\infty N_{jm}^* \left(t, X, Z\right) e^{-pt} dt$, p is the imaginary-significant parameter of Laplace transform.

A solution of Problem A_0^*. The solution of boundary problem (22)-(25) is:

$$N_{j0}^* \left(p, X, Z\right) = K_j C_{j0}^* \left(p, Z\right) \, sh \left(R \sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}} X \right) \Big/ sh \left(R \sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}} \right), j = \overline{1,3}. \tag{31}$$

We calculate

$$\left(\frac{\partial N_{i0}^* \left(p, X, Z\right)}{\partial X} \right)_{X=1} = R \sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_i}}} cth \left(R \sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_i}}} \right) K_i C_{i0}^* \left(p, Z\right) \tag{32}$$

than, substituting (30) and (31) into equation (26) we obtain:

$$\frac{\partial^2 C_{j0}^*}{\partial Z^2} - \gamma_j^2 \left(p\right) C_{j0}^* \left(p, Z\right) = 0 \tag{33}$$

where

$$\gamma_j^2(p) = \Gamma_j K_j \left(\frac{e_{inter_j}}{3K_j} \frac{R^2}{D_{intra_j}} p + R\sqrt{\frac{p}{D_{intra_j}}} cth \left(R\sqrt{\frac{p}{D_{intra_j}}} \right) - 1 \right);$$
$$\Gamma_j = \frac{3}{e_{\mathrm{inter}_j}} \frac{l^2}{\mathrm{R}^2} \frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{D}_{\mathrm{inter}_j}}.$$

The solution of equation (22) taking into account the boundary conditions (29) are as follows:

$$C_{j_0}^*(p, Z) = C_j^{in} \frac{1}{p} \frac{ch\left[\gamma_j(p) Z\right]}{ch\left[\gamma_j(p)\right]} = C_j^{in} \frac{1}{p} \frac{\cos\left[\gamma_j(p) Z\right]}{\cos\left[\gamma_j(p)\right]}. \tag{34}$$

The roots of transcendental equations $ch\left[\gamma_j(p)\right] = \cos\left[\gamma_j(\beta)\right] = 0$ are determined from transcendental equations $\gamma_j(\beta) = (2k-1)\pi/2,\ \mathrm{k} = \overline{1, \infty}$ or:

$$\beta^j ctg\left(\beta^j\right) - \frac{e_{\mathrm{inter}_j}}{3K_j}\left(\beta^j\right)^2 = 1 - \frac{1}{\Gamma_j K_j}\left(\frac{2k-1}{2}\pi\right)^2,\ \mathrm{k} = \overline{1, \infty}. \tag{35}$$

Using Heaviside's theorem on the decomposition of a rational complex expression into a series by the roots of the denominator and making a substitution $p = -D_{intra_j}\beta_j^2/R^2$, we obtain a formula for returning the Laplace image to the original (33):

$$C_{j_0}(t, Z) = C_j^{in}\left(1 + \sum_{s=1}^{\infty}\sum_{k=1}^{\infty} \frac{ch\left[\gamma_j(p) Z\right] \exp\left(p_{ks} t\right)}{p_{ks} \frac{d}{dp}\, ch\left[\gamma_j(p)\right]\big|_{p=p_{ks}}}\right);\ p_{ks} = -\frac{D_{intra_j}(\beta_{ks}^j)^2}{R^2}, \tag{36}$$

where β_{ks}^j are distinct positive roots of transcendental equations (34).

After simplifications we obtain:

$$C_{j_0}(t, Z) = C_j^{in}\left(1 + 2\left(\frac{R}{l}\right)^2 \frac{\mathrm{D}_{\mathrm{inter}_j}}{\mathrm{D}_{\mathrm{intra}_j}} \times \right.$$
$$\left. \times \sum_{s=1}^{\infty}\sum_{k=1}^{\infty} \frac{(2k-1)\pi\cos\left(\frac{2k-1}{2}\pi Z\right)\exp\left(-\frac{D_{intra_j}}{R^2}\left(\beta_{ks}^j\right)^2 t\right)}{(-1)^{\mathrm{s}}\left(\beta_{ks}^j\right)^2\left[\frac{3K_j}{\mathrm{e}_{\mathrm{inter}_j}}\left(\frac{1}{\sin^2\left(\beta_{ks}^j\right)} - \frac{ctg\left(\beta_{ks}^j\right)}{\beta_{ks}^j}\right) + 2\right]}\right). \tag{37}$$

Transforming formula (30) to a compact form we have:

$$N_{j_0}^*(p, X, Z) = C_{j_0}^*(p, Z)\ \frac{\sin(\beta X)}{\sin(\beta)} = \frac{C_j^{in}}{p} \frac{ch\left[\gamma_j(p) Z\right]}{ch\left[\gamma_j(p)\right]} \frac{\sin(\beta X)}{\sin(\beta)};\ i\beta = R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}$$

and as a result of applying to it the Heaviside theorem on the expansion into a series, we obtain a formula for calculating the Laplace original of the function $N_{j_0}(t, X, Z)$:

$$N_{s_1}(t, X, Z) = 1 + \sum_{n=1}^{\infty}\sum_{k=1}^{\infty} \frac{\sin(\beta X)\, ch\left[\gamma_{s_1}(p_{kn})Z\right] \exp\left(p_{kn_1} t\right)}{p_{kn_1}\sin(\beta)\, \frac{d}{dp}\, ch\left[\gamma_{s_1}(p) l\right]\big|_{p=p_{kn_1}=-\frac{D_{intra_{s_1}}\beta_{kn_1}^2}{R^2}}}. \tag{38}$$

After transformation and going to the function $Q_{j_0}(t,X,Z)$ to describe the concentration distributions of the adsorbed components in the nanopores of the particles:

$$Q_{j_0}(t,Z) = C_j^{in}\left(1+2\left(\frac{R}{l}\right)^2\frac{\mathrm{D}_{\mathrm{inter}_j}}{\mathrm{D}_{\mathrm{intra}_j}}\times\right.$$
$$\left.\times\sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{(2k-1)\,\pi\sin\left(\beta_{ks}^{j}X\right)\cos\left(\frac{2k-1}{2}\pi Z\right)\exp\left(-\frac{D_{intra_j}}{R^2}(\beta_{ks}^{j})^2 t\right)}{(-1)^{\mathrm{n}}\,(\beta_{ks}^{j})^2X\sin\left(\beta_{ks}\right)\left[\frac{3K_j}{\mathrm{e}_{\mathrm{inter}_j}}\left(\frac{1}{\sin^2(\beta_{ks}^{j})}-\frac{ctg\left(\beta_{ks}^{j}\right)}{\beta_{ks}^{j}}\right)+2\right]}\right). \tag{39}$$

A solution of Problem A_m. A solution of boundary problem (27), (28) is

$$N_{j_m}^{*}\left(p,X,Z\right)=\left(K_jC_{j_m}^{*}\left(p,Z\right)-F_{j_m}^{*}\left(p,Z\right)\right)\frac{sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}X\right)}{sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}\right)},\, j=\overline{1,3} \tag{40}$$

From (39) at $X=1$ we obtain:

$$\left(\frac{\partial N_{i_m}^{*}\left(p,X,Z\right)}{\partial X}\right)_{X=1}=R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_i}}}cth\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_i}}}\right)\left(K_jC_{j_m}^{*}\left(p,Z\right)-F_{j_m}^{*}\left(p,Z\right)\right).$$

By substituting $N_{j_m}^{*}\,|_{X=1}$ and $\left.\frac{\partial N_{j_m}^{*}}{\partial X}\right|_{X=1}$ in equation (38) we obtain:

$$\frac{d^2\,C_{j_m}^{*}}{d\,Z^2}-\gamma_j^2\left(p\right)C_{j_m}^{*}=-\Phi_{j_m}^{*}\left(p,Z\right) \tag{41}$$

here $\Phi_{j_m}^{*}\left(p,Z\right)=\Gamma_j\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_i}}}cth\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_i}}}\right)-1\right)F_{j_m}^{*}\left(p,Z\right),\, m=\overline{1,\infty}$.

A solution of the inhomogeneous problem (40), (29) are as follows [15]:

$$C_{j_m}^{*}\left(p,X,Z\right)=-\int_0^1\mathcal{K}_j^{*}\left(p,Z,\xi\right)\Phi_{j_m}^{*}\left(p,\xi\right)d\xi, \tag{42}$$

where the fundamental function of Cauchy's influence $\mathcal{K}_j^{*}\left(p,Z,\xi\right)$, which is determined as follows:

$$\mathcal{K}_j^{*}\left(p,Z,\xi\right)=\begin{cases}\mathcal{K}_j^{-*}\left(p,Z,\xi\right)=d_1Ah\,\gamma_jZ+e_1sh\,\gamma_jZ, 0<Z<\xi<1\\ \\ \mathcal{K}_j^{+*}\left(p,Z,\xi\right)=d_2ch\gamma_jZ+e_2sh\gamma_jZ, 0<\xi<Z<1\end{cases}. \tag{43}$$

All the coefficients $d_s, e_s, s=\overline{1,2}$ in expressions (44) are determined by conditions [15]:

$$\begin{cases}\mathcal{K}_j^{*}\left(p,Z,\xi\right)\big|_{Z=\xi+0}-\mathcal{K}_j^{*}\left(p,Z,\xi\right)\big|_{Z=\xi-0}=0\\ \\ \frac{d}{dZ}\mathcal{K}_j^{*}\left(p,Z,\xi\right)\big|_{Z=\xi+0}-\frac{d}{dZ}\mathcal{K}_j^{*}\left(p,Z,\xi\right)\big|_{Z=\xi-0}=1\end{cases} \tag{44}$$

and an additional condition (boundary condition at $Z = 1$):

$$\mathcal{K}_j^{+*}\big|_{Z=1} \equiv \left[d_2 ch\gamma_j Z + e_2 sh\gamma_j Z\right]_{Z=1} = 0. \tag{45}$$

Consistently, applying conditions (44)-(46) as a result, the Cauchy function $\mathcal{K}_j^*(p, Z, \xi)$ is fully determined in the following form:

$$\mathcal{K}_j^*(p, Z, \xi) = -\frac{1}{\gamma_j}\begin{cases} \dfrac{sh\left(\gamma_j(1-\xi)\right)\cdot ch\left(\gamma_j Z\right)}{ch\left(\gamma_j\right)}, 0 < Z < \xi < 1 \\ \\ \dfrac{sh\left(\gamma_j(1-Z)\right)\cdot ch\left(\gamma_j \xi\right)}{ch\left(\gamma_j\right)}, 0 < \xi < Z < 1 \end{cases} \tag{46}$$

Defining another function of influence:

$$\mathcal{H}_j^*(p, Z, \xi) = -\frac{R\sqrt{\dfrac{p}{\mathrm{D}_{\mathrm{intra}_i}}}cth\left(R\sqrt{\dfrac{p}{\mathrm{D}_{\mathrm{intra}_i}}}\right)}{\gamma_j}\mathcal{K}_j^*(p, Z, \xi) \tag{47}$$

solution (44) will take the following form :

$$C_{j_m}^*(p, X, Z) = -\Gamma_j\int_0^1\left(\mathcal{H}_j^*(p, Z, \xi) - \mathcal{K}_j^*(p, Z, \xi)\right)F_{j_m}^*(p, \xi)\,d\xi. \tag{48}$$

The transition to originals. We carry out the transition to the originals $C_{j_m}(t, X, Z)$ using the formula:

$$C_{j_m}(t, X, Z) = -\Gamma_j\int_0^1 L^{-1}\left[\mathcal{H}_j^*(p, Z, \xi) - \mathcal{K}_j^*(p, Z, \xi)\right] * F_{j_m}(t, \xi)\,d\xi \tag{49}$$

where $L^{-1}[...]$ - is the designation of the Laplace inverse transform operator, $*$ is the image convolution operator. In the final form, after calculating the originals, formula (47) takes the form:

$$\begin{gathered} C_{j_m}(t, X, Z) = -\frac{3}{e_{\mathrm{inter}_j}}\frac{l^2}{\mathrm{R}^2}\frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{D}_{\mathrm{inter}_j}}\times \\ \times\int_0^t\left(\begin{array}{c}\int_Z^1\left(\mathcal{H}_j^-(t-\tau, Z, \xi) - \mathcal{K}_j^-(t-\tau, Z, \xi)\right)F_{j_m}(\tau, \xi)\,d\xi + \\ \\ +\displaystyle\int_0^Z\left(\mathcal{H}_j^+(t-\tau, Z, \xi) - \mathcal{K}_j^+(t-\tau, Z, \xi)\right)F_{j_m}(\tau, \xi)\,d\xi\end{array}\right)d\tau \end{gathered}, \tag{50}$$

were $\mathcal{H}_j^-(t-\tau, Z, \xi), \mathcal{K}_j^-(t-\tau, Z, \xi)$, $\mathcal{H}_j^+(t-\tau, Z, \xi), \mathcal{K}_j^+(t-\tau, Z, \xi)$ are the components of influence functions (45), (47), the calculation algorithms of which are given below.

Applying to the components of the influence functions (45), (47) the Heaviside theorem on the development of a rational complex expression into a convergent series, we obtain:

$$\begin{gathered} L^{-1}\left[\frac{f_j^h(p)}{\gamma_j(p)\,sh\left[\gamma_j(p)\right]ch\left[\gamma_j(p)\right]}\right] = \sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{f_j^h\left(\beta_{ks}^j\right)e^{\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\beta_{ks}^j\right)^2 t}}{\omega_j^1\left(\beta_{ks}^j\right)} + \\ +\sum_{s_1=1}^{\infty}\frac{f_j^h\left(\mu_{s_1}^j\right)e^{\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\mu_{s_1}^j\right)^2 t}}{\nu_j^2\left(\mu_{s_1}^j\right)} + \sum_{k_1=1}^{\infty}\frac{f_j^h\left(\eta_{k_1}^j\right)e^{\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\eta_{k_1}^j\right)^2 t}}{\omega_j^2\left(\eta_{k_1}^j\right)} \end{gathered} \tag{51}$$

where $f_j^h, h=\overline{1,4}$ determine, respectively, the numerators of the components $\mathcal{H}_j^{\pm}(t-\tau,Z,\xi)$ - the influence functions (46).

Calculate the denominators in the expressions of the sums of each of the three terms of the right-hand side of formula (50):

$$\omega_j^1\left(\beta_{ks}^j\right) \equiv \gamma_j\left(p\right) sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}\right)\frac{d}{dp}ch\left[\gamma_j(p)\right]\Big|_{p=\beta_{ks}^j} =$$

$$= -\gamma_j\left(\beta_{ks}^j\right)\sin\left(\beta_{ks}^j\right)\frac{(-1)^k\left(\beta_{ks}^j\right)^2}{2k-1}\left[\frac{3K_j}{\mathrm{e}_{\mathrm{inter}_j}}\left(\frac{1}{\sin^2(\beta_{ks}^j)}-\frac{ctg(\beta_{ks}^j)}{\beta_{ks}^j}\right)+2\right] \tag{52}$$

where $\left\{\beta_{ks}^j\right\}, k, s=\overline{1,\infty}$ - set of roots of transcendental equation (34):

$$\nu_j^1\left(\mu_{s_1}^j\right) \equiv \gamma_j\left(p\right) ch\left[\gamma_j\left(p\right)\right]\frac{d}{dp}sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}\right)\Bigg|_{p=-\frac{\mathrm{D_{intra}}}{R^2}\left(\mu_{s_1}^j\right)^2} =$$

$$= \gamma_j\left(\mu_{s_1}^j\right)\cos\left[\gamma_j\left(\mu_{s_1}^j\right)\right](-1)^{s_1}\frac{R^2}{2\mathrm{D}_{\mathrm{intra}_j}\mu_{s_1}^j}\Big|_{\mu_{s_1}^j=\pi s_1};$$

$$\omega_j^2\left(\eta_{k_1}^j\right) \equiv sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}\right) ch\left[\gamma_j(p)\right]\frac{d}{dp}\gamma_j\left(p\right)\Bigg|_{p=-\frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{R}^2}\left(\mu_{k_1}^j\right)^2} =$$

$$= -\frac{l}{2R}\sqrt{\frac{3K_j}{e_{\mathrm{inter}_j}}\frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{D}_{\mathrm{inter}_j}}}\frac{\dfrac{ctg\left(\eta_{k_1}^j\right)}{\eta_{k_1}^j}-\dfrac{1}{\sin^2\eta_{k_1}^j}+\dfrac{2e_{\mathrm{inter}_j}}{3}}{\sqrt{\dfrac{e_{\mathrm{inter}_j}}{3K_j}+\dfrac{ctg\left(\eta_{k_1}^j\right)}{\eta_{k_1}^j}-\dfrac{1}{\left(\eta_{k_1}^j\right)^2}}}\sin\left(\eta_{k_1}^j\right)\cos\left[\gamma_j\left(\eta_{k_1}^j\right)\right],$$

where $\left\{\eta_{k_2}^j\right\}_{k_2=\overline{1,\infty}}^{j=\overline{1,3}}$ is the set of roots of transcendental equation:

$$\frac{e_{\mathrm{inter}_j}}{3K_j}\left(\mu^j\right)^2-\mu^j ctg\ \left(\mu^j\right)+1=0,\ \gamma_j^1\left(p\right)=0,\ R\sqrt{\frac{p}{D_{intra_j}}}=i\mu^j$$

As a result, we obtain the following expressions of the originals:

$$\mathcal{H}_j^-(t,Z,\xi)=L^{-1}\left[\mathcal{H}_j^{-*}(p,Z,\xi)\right]=$$

$$=\sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{\beta_{ks}^j\cos\left(\beta_{ks}^j\right)\sin\left(\gamma_j\left(\beta_{ks}^j\right)(1-\xi)\right)\cdot\cos\left(\gamma_j\left(\beta_{ks}^j\right)Z\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\beta_{ks}^j\right)^2t}}{\omega_j^1\left(\beta_{ks}^j\right)}+$$

$$+\sum_{s_1=1}^{\infty}\frac{\mu_{s_1}^j\cos\left(\mu_{s_1}^j\right)\sin\left(\gamma_j\left(\mu_{s_1}^j\right)(1-\xi)\right)\cdot\cos\left(\gamma_j\left(\mu_{s_1}^j\right)Z\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\mu_{s_1}^j\right)^2t}}{\nu_j^2\left(\mu_{s_1}^j\right)}$$

$$+\sum_{k_1=1}^{\infty}\frac{\eta_{k_1}^j\cos\left(\eta_{k_1}^j\right)\sin\left(\gamma_j\left(\eta_{k_1}^j\right)(1-\xi)\right)\cdot\cos\left(\gamma_j\left(\eta_{k_1}^j\right)Z\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\eta_{k_1}^j\right)^2t}}{\omega_j^2\left(\eta_{k_1}^j\right)};$$

$$\mathcal{H}_j^+(t,Z,\xi)\equiv L^{-1}\left[\mathcal{H}_j^{+*}(p,Z,\xi)\right]=$$

$$=\sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{\beta_{ks}^j\cos\left(\beta_{ks}^j\right)\sin\left(\gamma_j\left(\beta_{ks}^j\right)(1-Z)\right)\cdot\cos\left(\gamma_j\left(\beta_{ks}^j\right)\xi\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\beta_{ks}^j\right)^2t}}{\omega_j^1\left(\beta_{ks}^j\right)}+$$

$$+\sum_{s_1=1}^{\infty}\frac{\mu_{s_1}^j\cos\left(\mu_{s_1}^j\right)\sin\left(\gamma_j\left(\mu_{s_1}^j\right)(1-Z)\right)\cdot\cos\left(\gamma_j\left(\mu_{s_1}^j\right)\xi\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\mu_{s_1}^j\right)^2t}}{\nu_j^2\left(\mu_{s_1}^j\right)}$$

$$+\sum_{k_1=1}^{\infty}\frac{\eta_{k_1}^j\cos\left(\eta_{k_1}^j\right)\sin\left(\gamma_j\left(\eta_{k_1}^j\right)(1-Z)\right)\cdot\cos\left(\gamma_j\left(\eta_{k_1}^j\right)\xi\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\eta_{k_1}^j\right)^2t}}{\omega_j^2\left(\eta_{k_1}^j\right)}$$

Next, we find the components $\mathcal{K}_j(t,Z,\xi)$. We have:

$$L^{-1}\left[\frac{g_j^h(p)}{\gamma_j(p)\,ch\left[\gamma_j(p)\right]}\right]=\sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{g_j^h\left(\beta_{ks}^j\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\beta_{ks}^j\right)^2t}}{\tilde{\omega}_j^1\left(\beta_{ks}^j\right)}+\sum_{k_1=1}^{\infty}\frac{g_j^h\left(\eta_{k_1}^j\right)e^{\frac{\mathrm{D_{intra}}_j}{R^2}\left(\eta_{k_1}^j\right)^2t}}{\tilde{\omega}_j^2\left(\eta_{k_1}^j\right)}\qquad(53)$$

where $g_j^h(p)$ determine $\mathcal{K}_j^+(t-\tau,Z,\xi)\,,\mathcal{K}_j^+(t-\tau,Z,\xi)$ are the components of influence functions (45).

We calculate the denominators in the expressions of the sums of each of the two terms of the right part of formula (51):

$$\tilde{\omega}_j^1\left(\beta_{ks}^j\right) \equiv \gamma_j\left(p\right)\frac{d}{dp}ch\left[\gamma_j(p)\right]\Big|_{p=\beta_{ks}^j} =$$

$$= i\gamma_j\left(\beta_{ks}^j\right)\frac{(-1)^k\beta_{ks}^{j2}}{2k-1}\left[\frac{3K_j}{\mathrm{e}_{\mathrm{inter}_j}}\left(\frac{1}{\sin^2(\beta_{ks}^j)}-\frac{ctg(\beta_{ks}^j)}{\beta_{ks}^j}\right)+2\right];$$

$$\tilde{\omega}_j^2\left(\eta_{k_1}^j\right) = ch\left[\gamma_j(p)\right]\frac{d}{dp}\gamma_j\left(p\right)\Big|_{p=-\frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{R}^2}\mu_{k_1}^j} = \qquad ,$$

$$= i\frac{l}{2R}\sqrt{\frac{3K_j}{e_{\mathrm{inter}_j}}\frac{\mathrm{D}_{\mathrm{intra}_j}}{\mathrm{D}_{\mathrm{inter}_j}}}\cdot\frac{\dfrac{ctg\left(\eta_{k_1}^j\right)}{\eta_{k_1}^j}-\dfrac{1}{\sin^2\eta_{k_1}^j}+\dfrac{2e_{\mathrm{inter}_j}}{3}}{\sqrt{\dfrac{e_{\mathrm{inter}_j}}{3K_j}+\dfrac{ctg\left(\eta_{k_1}^j\right)}{\eta_{k_1}^j}-\dfrac{1}{\left(\eta_{k_1}^j\right)^2}}}\cos\left[\gamma_j\left(\eta_{k_1}^j\right)\right]$$

The expressions of originals are:

$$\mathcal{K}_j^-\left(t,Z,\xi\right) = L^{-1}\left[\mathcal{K}_j^{-*}\left(p,Z,\xi\right)\right] =$$

$$= -\sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{\sin\left(\gamma_j\left(\beta_{ks}^j\right)(1-\xi)\right)\cdot\cos\left(\gamma_j\left(\beta_{ks}^j\right)Z\right)e^{-\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\beta_{ks}^j\right)^2t}}{\tilde{\omega}_j^1\left(\beta_{ks}^j\right)} -$$

$$-\sum_{k_1=1}^{\infty}\frac{\sin\left(\gamma_j\left(\eta_{k_1}^j\right)(1-\xi)\right)\cdot\cos\left(\gamma_j\left(\eta_{k_1}^j\right)Z\right)e^{-\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\eta_{k_1}^j\right)^2t}}{\tilde{\omega}_j^2\left(\eta_{k_1}^j\right)};$$

$$\mathcal{K}_j^+\left(t,Z,\xi\right) = L^{-1}\left[\mathcal{K}_j^{+*}\left(p,Z,\xi\right)\right] =$$

$$= -\sum_{s=1}^{\infty}\sum_{k=1}^{\infty}\frac{\sin\left(\gamma_j\left(\beta_{ks}^j\right)(1-Z)\right)\cdot\cos\left(\gamma_j\left(\beta_{ks}^j\right)\xi\right)e^{-\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\beta_{ks}^j\right)^2t}}{\tilde{\omega}_j^1\left(\beta_{ks}^j\right)} +$$

$$-\sum_{k_1=1}^{\infty}\frac{\sin\left(\gamma_j\left(\eta_{k_1}^j\right)(1-Z)\right)\cdot\cos\left(\gamma_j\left(\eta_{k_1}^j\right)\xi\right)e^{-\frac{\mathrm{D}_{\mathrm{intra}_j}}{R^2}\left(\eta_{k_1}^j\right)^2t}}{\tilde{\omega}_j^2\left(\eta_{k_1}^j\right)}$$

$N_{j_m}\left(t,X,Z\right)$ is calculated on basis of formula (51). We obtain:

$$L^{-1}\left[N_{j_m}^*(p,X,Z)\right] = L^{-1}\left[K_jC_{j_m}^*\left(p,Z\right)-F_{j_m}^*\left(p,Z\right)\right]*L^{-1}\left[\frac{sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}X\right)}{sh\left(R\sqrt{\frac{p}{\mathrm{D}_{\mathrm{intra}_j}}}\right)}\right]. \quad (54)$$

We calculate the original of function $\Psi^*_{jm}(p,X) = sh\left(R\sqrt{\frac{p}{\mathrm{D_{intra}}_j}}X\right) \Big/ sh\left(R\sqrt{\frac{p}{\mathrm{D_{intra}}_j}}\right)$:

$$L^{-1}\left[\Psi^*_{jm}(p,X)\right] = \sum_{k_2=0}^{\infty} \frac{sh\left(R\sqrt{\frac{p}{\mathrm{D_{intra}}_j}}X\right)}{\frac{d}{dp}\left(sh\left(R\sqrt{\frac{p}{\mathrm{D_{intra}}_j}}\right)\right)_{p=p^j_{k_2}}} \exp\left(p^j_{k_2}t\right) = \qquad (55)$$

$$= 2\sum_{k_2=0}^{\infty} \frac{\mathrm{D_{intra}}_j}{\mathrm{R}^2} \frac{k_2\pi\cdot\sin(k_2\pi X)}{(-1)^{k_2+1}} \exp\left(-\frac{\mathrm{D_{intra}}_j}{\mathrm{R}^2}k_2^2\pi^2 t\right)$$

Here $p^j_{k_2} = -D_{intra_j}\dfrac{\pi^2 k_2^2}{R^2}$, $k_2 = \overline{0,\infty}$ are the roots of the equation $sh\left(R\sqrt{\dfrac{p}{\mathrm{D_{intra}}_j}}\right) = 0$. Applying formula (50) to (49) one calculus the original $N_{jm}(t,X,Z)$:

$$N_{jm}(t,X,Z) = L^{-1}\left[\left(K_j C^*_{jm}(p,Z) - F^*_{jm}(p,Z)\right) * \Psi_j(p,Z)\right] =$$

$$= \int_0^t \left(K_j C_{jm}(t-\tau,Z) - F_{jm}(t-\tau,Z)\right)\times \qquad (56)$$

$$\times\left(2\frac{\mathrm{D_{intra}}_j}{\mathrm{R}^2}\sum_{k_2=0}^{\infty}\frac{\pi k_2\cdot\sin(k_2\pi X)}{(-1)^{k_2+1}}\exp\left(-\frac{\mathrm{D_{intra}}_j}{\mathrm{R}^2}k_2^2\pi^2 t)\right)\right)d\tau$$

Returning to the functions Q_{jm}, we obtain:

$$Q_{jm}(t,X,Z) = \int_0^t \left(K_j C_{jm}(t-\tau,Z) - \sum_{s=0}^{m-1}\sum_{k=1}^{3}\frac{K_j K_k}{K_1^2}C_{js}(t-\tau,Z)\,C_{k_{m-1-s}}(t-\tau,Z)\right)\times$$

$$\times\left(2\frac{\mathrm{D_{intra}}_j}{\mathrm{R}^2}\sum_{k_2=0}^{\infty}\frac{\pi k_2\cdot\sin(k_2\pi X)}{(-1)^{k_2+1}X}\exp\left(-\frac{\mathrm{D_{intra}}_j}{\mathrm{R}^2}k_2^2\pi^2 t)\right)\right)d\tau,\ j=\overline{1,3}. \qquad (57)$$

The following theorem holds.

Theorem 1. *If the given and unknown functions of boundary-value problems* (23)-(23), *are Laplace pre-images with respect to the time variable* t *and the unique solvability conditions of boundary-value problems* A_0 *and* A_m *of the Laplace images are satisfied, then the solutions to the boundary-value problems* A_0 *and* A_m, *exist, are unique, and are determined by formulas* (37),(39) *and* (51),(57), *which constitute the solution of initial nonlinear boundary-value problem* (1)-(6).

2 Simulation and Discussion

The purpose of computer modeling was to study the capabilities of the model proposed for further use in technologies for cleaning carbon emissions into the atmosphere by energy and

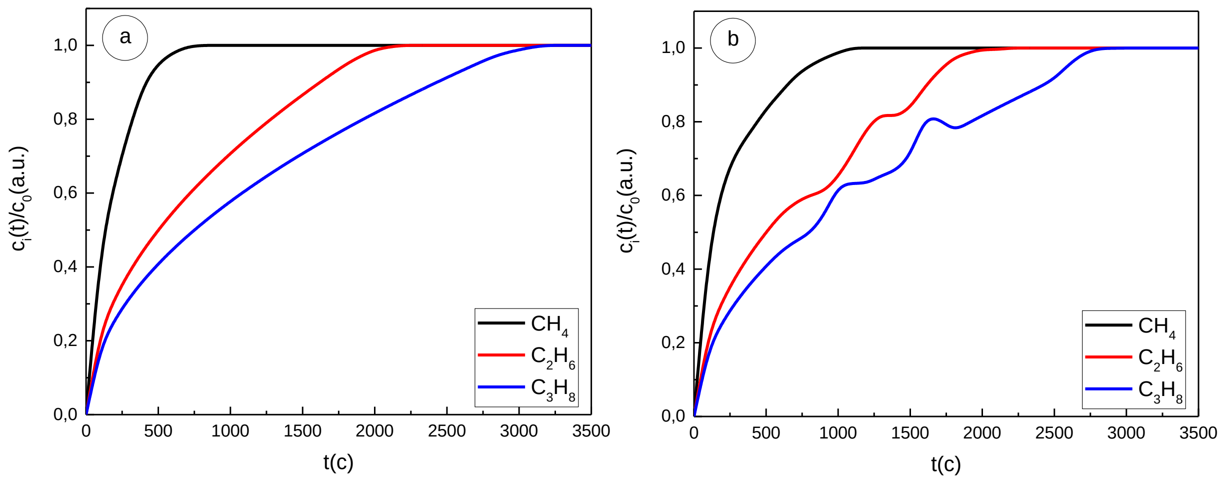

Figure 1: Breakthrough curves ($ci(t)/c0$, i = 1,2,3) for three-component adsorption for a mixture of methane (CH_4, i = 1), ethane (C_2H_6, i = 2), propane (C_3H_8, i = 3) taken from different mass ratios in the input mixture: (80%, 15%, 5%) (a), (35%, 35%, 30%) (b)

transport facilities (propane, CO_2 and other combustion products). This is one of the key ways to solve the problem of global warming and create a safe energy strategy [2]. Propane was chosen as an adsorbent, the volume of which covers about 30% of the total gas flow leaving the car's engine. Using the developed mathematical theory and technology oriented to parallel multicore computer calculations, the modeling and calculation of concentration dependencies of three-component adsorption and desorption curves in nanoporous catalytic layers are carried out. Computational experiments were performed for the experimental sample [7, 10, 12, 14].

3 Conclusions

High-performance methods and computational technologies for modeling non-isothermal gas adsorption in nanoporous solid for three-component adsorption equilibrium have been developed. On their basis, new nonlinear mathematical models have been constructed, including the balance equations of adsorption/desorption taking into account the interaction of intracrystalite space (micro flows) and intercrystallite space (macro flows). Effective schemes for parallelizing and linearizing nonlinear models were developed on basis of the equilibrium function decomposition into a series at the point of phase transition temperature as a small parameter. High-speed analytical and numerical solutions of mathematical models using the Heaviside operational method, their algorithmic and software implementation is implemented, which ensures efficient parallelization of computational processes for multicore computers and increased computational speed have been constructed.

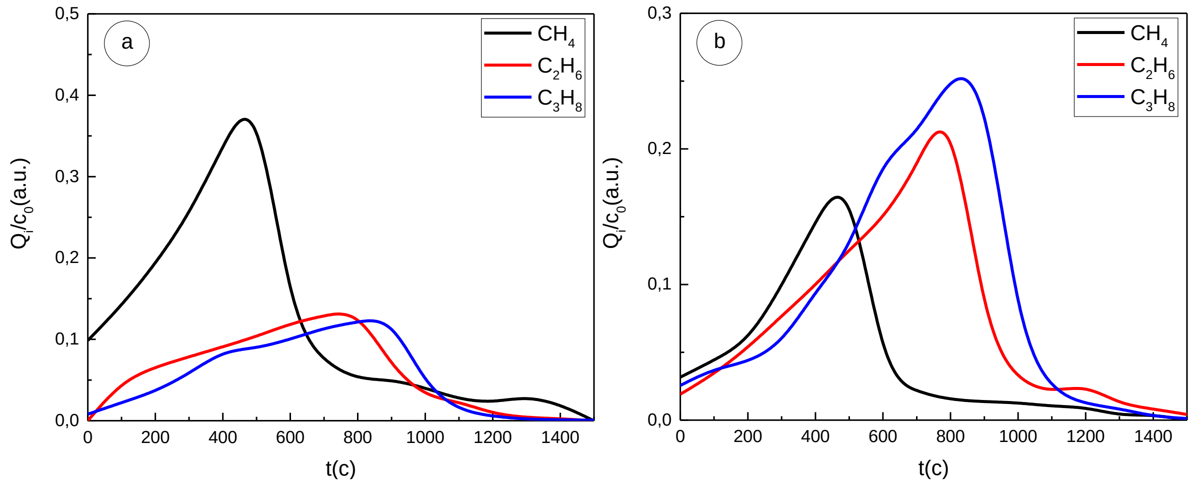

Figure 2: Desorption curves of gases in zeolite nanopores ($Qi(t)/c0$, i = 1,2,3) for a mixture of methane (CH_4, i = 1), ethane (C_2H_6, i = 2), propane (C_3H_8, i = 3) taken in different mass ratios in the input mixture: (80%, 15%, 5%) (a), (35%, 35%, 30%) (b)

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Петрик М.Р., Бойко І.В., Шинкарик М.І., Петрик О.Ю. *Нелінійна модель компетитивної дифузії для трикомпонентної адсорбції з використанням рівноважної ізотерми Ленгмюра* // Буковинський матем. журнал — 2021. — Т.9, №1. — С. 64–78.

Наведені основи математичного моделювання неізотермічної трикомпонентної компетитивної адсорбції газу в нанопористому середовищі з використанням рівноваги Ленгмюра. Запропоновано високоефективні аналітичні розв'язки для розвиненої моделі адсорбції з використанням операційного методу Гевісайда та інтегрального перетворення Лапласа.

Наведено результати комп'ютерного моделювання на основі високошвидкісних обчислень на багатоядерних комп'ютерах.