

**MODELLING THE PROCESS OF AIR OXYGENATION
BY NITROGEN ADSORPTION IN A PRESSURE
SWING ADSORPTION UNIT**

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Abstract: A mathematical model and algorithm of solving equations of air oxygenation dynamics model for a two-adsorber unit of pressure swing adsorption with vacuum desorption for people with chronic obstructive lung disease, have been developed. Mass- and heat-exchange processes that occur during nitrogen adsorption from gas-air mixture with the help of block zeolite adsorbent have been mathematically modeled.

Symbols

a_i – concentration in adsorbent, mole/m ³ ;	n – degree index in equations of micropore volumetric filling theory;
a^* – equilibrium adsorption value, mole/m ³ ;	n_c – number of adsorption-desorption cycles;
A – nitrogen constant;	P – pressure, Pa;
B – coefficient of equations of micropore volumetric filling theory, K ⁻² ;	P^* – saturation pressure, Pa;
C_p – heat capacity, J/(kg·K);	R – universal gas constant; J/(mole·K);
C – nitrogen constant;	S – area, m ² ;
c – concentration in gas phase, mole/m ³ ;	S_a – surface area of adsorbent’s transporting pores, m ² ;
$c_{O_2}^{vol}$ – oxygen concentration in gas phase at the unit’s outlet, m ³ /m ³ , % vol.;	t – time, s;
D_{int} – internal diameter of adsorber, m;	T – temperature, K;
D_g – diffusion coefficient in gas phase, m ² /s;	V – volume, m ³ ;
d_e – equivalent diameter of adsorbent’s transporting pores, m;	V_{work} – adsorber’s working volume, m ³ ;
E_0 – characteristic adsorption energy, J/mole;	W – volume flow rate, m ³ /s;
F – nitrogen constant;	W_0 – maximum adsorption volume, sm ³ /g;
h – thermal effect, J/mole;	w – speed of gas flow, m/s;
h_x – coordinate pitch distance in finite elements grid, m;	α – heat exchange coefficient, Wt/(m ² ·K);
H – height of adsorbent layer, m;	β – external mass transfer coefficient, m/s;
m – mass, kg;	γ – condensation-evaporation heat, J/kg;
M – molar mass, kg/kmole;	δ – fixed precision of computation;
N – number of grid cells;	ε – volume fraction of transporting pores (porosity coefficient);
N_{cons} – power consumption, Wt;	θ – backwashing coefficient;
	η – kinematic viscosity of air, m ² /s;
	λ – thermal conductivity coefficient, Wt/(m·K);

μ – dynamic viscosity of air, Pa·s;
 v – molar volume, mole/m³;
 ρ – density, kg/m³;
 σ – specific surface area of adsorbent's transporting pores, m²/m³;
 τ_t – time pitch distance, s;
 φ – thermal coefficient of maximum adsorption;
 ψ – affine property coefficient;

Indices

a – adsorbent (in adsorbent);
 ad – adsorption;

c – cycle;
 cr – critical;
 des – desorption;
 e – equivalental;
 g – gas phase (in gas phase);
 giv – given;
 in – inlet;
 N₂ – nitrogen;
 O₂ – oxygen;
 pr – product;
 rev – reverse;
 tr – transporting pores;
 v – iteration number.

Introduction

Rapid development of pressure swing adsorption (PSA) technologies allowed for the development of highly effective and, at the same time, simple and cost-efficient units for air oxygenation that can be competently used for medical purposes [1–4]. PSA units can also be implemented for gas-air mixture decontamination [5, 6].

The work of PSA unit is based on the principle of cycled process alternation of nitrogen adsorption from gas-air mixture and nitrogen desorption from adsorbent in parallel adsorbers. Thus a continuous flow of oxygenated air is formed at the PSA unit's outlet (Fig. 1).

At inlet the flow of gas-air mixture is compressed by compressor 1 up to P_{ad} pressure and enters adsorber 2a, which is filled with block zeolite adsorbent. Nitrogen is adsorbed by the adsorbent under P_{ad} pressure during time interval from 0 till $t_c/2$ and this way the gas-air mixture is oxygenated (direct flow at the unit's outlet). The adsorption process is carried with the emission of heat, which is accumulated in the adsorbent and is used for its subsequent regeneration.

A portion of oxygenated gas-air mixture is throttled down through valve 5 till pressure $P = P_{des}$, created by vacuum pump 7, and is directed in counter-flow into adsorber 2b for nitrogen desorption from the adsorbent during time interval from $t_c/2$ till t_c . As a result, adsorbent regeneration is carried out in adsorber 2b.

When closing valves 3a and 4b and opening valves 3b and 4a, nitrogen desorption takes place in adsorber 2a and nitrogen adsorption takes place in adsorber 2b. When valves turn in reverse positions, the cycle is repeated.

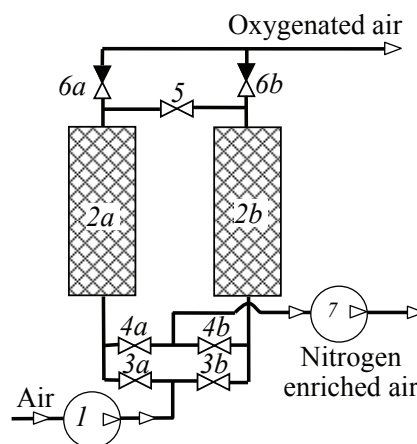


Fig. 1. PSA unit diagram:

1 – compressor; 2a, 2b – adsorbers; 3a, 3b, 4a, 4b – controlled valves; 5 – throttling valve; 6a, 6b – check valves; 7 – vacuum pump

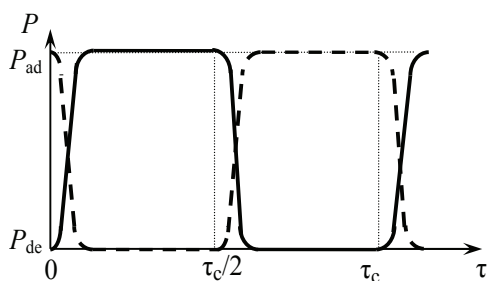


Fig. 2. PSA unit operation cyclogram:

— – 2a; - - - - 2b

Mathematical Description of Air Oxygenation Process

Our research has shown that the most promising type of oxygenation process instrumentation involves zeolite adsorbent in the form of porous solid block with transporting pores of $d_e \leq 0,5 \times 10^{-3}$ m in equivalent diameter (adsorption volume limit is $0,195 \text{ sm}^3 \cdot \text{kg}^{-1}$ and specific surface area of transporting pores is $124,300 \text{ m}^2/\text{m}^3$). When used for a long term, the zeolite adsorbent solid block does not wear off during cyclic processes of adsorption and desorption (the block's ultimate strength equals $\sim 54 \times 10^5 \text{ Pa}$) [7].

When the zeolite adsorbent adsorbs nitrogen the following mass- and heat exchange processes occur: a) nitrogen diffusion in gas phase; b) heat emission in gas flow and adsorbent; c) external nitrogen mass exchange and heat exchange between gas and solid phases; d) nitrogen adsorption in solid zeolite adsorbent micropores with heat emission and nitrogen desorption from micropores with heat consumption.

When researching and modeling mass- and heat-exchange processes that accompany adsorption of gases by microporous adsorbents, the theory of micropore volumetric filling, developed by the Academician M.M. Dubinin [8] and advocated by many other scientists [9–13], is most frequently used. According to this theory, adsorbent's micropores represent spatial regions which size is proportional to the adsorbed molecules. The adsorption field has effect over the entire space of adsorbent's micropores, and adsorption within the micropores is determined by the filling of adsorption space. In this case the volume of micropores becomes the main geometric parameter that characterizes a microporous adsorbent, and hence, the notion of adsorption volume limit of micropores is introduced.

The process of external mass transfer imposes certain limitations on air oxygenation during nitrogen adsorption by microporous zeolite adsorbent; it depends on coefficient β and value $a_i^*(c, T_g)$ of equilibrium nitrogen concentration in solid phase [9]. Taking this into consideration, when deriving equations for mass- and heat-exchange during nitrogen adsorption by block zeolite adsorbent we have assumed the following: 1) a solid porous zeolite block with the volume of transporting pores $\varepsilon = 0,394$ is used as an adsorbent; the volume of transporting pores V_{tr} for gas phase in a grid cell is calculated as $V_{tr} = S_{tr} \Delta x$, where S_{tr} is an area of transporting pores at section x ; 2) the height of adsorbent H in the adsorber is divided into N grid cells, in each of which the concentration a_i of adsorbed nitrogen and temperature T_{ai} depend on time, i.e. $a_i = a_i(t)$, $T_{ai} = T_{ai}(t)$, $i = \overline{1, N}$; 3) adsorption of oxygen from gas-air mixture is not considered; 4) the longitudinal nitrogen diffusion coefficient D_g in gas phase depends on the temperature T_g of gas-air flow.

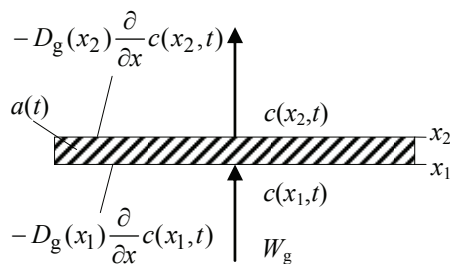


Fig. 3. To the derivation of equation of nitrogen diffusion in gas phase

We shall formulate equations of the mathematical model of air oxygenation involving nitrogen adsorption (desorption) from gas-air mixture with the use of solid porous zeolite adsorbent, and mass- and heat exchange processes in gas and solid phases (Fig. 3.)

1. Nitrogen diffusion in gas-air mixture over the adsorbent's height.

Implementing the laws of conservation, we shall formulate an equation of mass

balance in a grid cell over the adsorbent's height (x_1, x_2) in a certain time interval (t_1, t_2) [14]:

$$W_g \int_{t_1}^{t_2} [c(x_1, t) - c(x_2, t)] dt + S_{tr} \int_{t_1}^{t_2} \left[(-D_g(x_1)) \frac{\partial}{\partial x} c(x_1, t) - (-D_g(x_2)) \frac{\partial}{\partial x} c(x_2, t) \right] dt - \\ - V_{ai} [a_i(t_2) - a_i(t_1)] = S_{tr} \int_{x_1}^{x_2} [c(x, t_2) - c(x, t_1)] dx,$$

where the number i of adsorbent layer corresponds to the interval (x_1, x_2) .

We shall assume that function $c(x, t)$ has continuous derivatives $\frac{\partial c}{\partial t}$ and $\frac{\partial^2 c}{\partial x^2}$.

Using the mean value theorem we obtain the following equality:

$$-W_g \frac{[c(x_2, t) - c(x_1, t)]}{\Delta x} \Big|_{t_3 \in (t_1, t_2)} \Delta t \Delta x + S_{tr} \frac{\left[D_g(x_2) \frac{\partial}{\partial x} c(x_2, t) - D_g(x_1) \frac{\partial}{\partial x} c(x_1, t) \right]}{\Delta x} \Big|_{t_4 \in (t_1, t_2)} \Delta t \Delta x - \\ - \frac{V_{ai}}{\Delta x} \frac{[a_i(t_2) - a_i(t_1)]}{\Delta t} \Delta t \Delta x = S_{tr} \frac{[c(x, t_2) - c(x, t_1)]}{\Delta t} \Big|_{x_3 \in (x_1, x_2)} \Delta x \Delta t,$$

where $\Delta x = (x_2 - x_1)$, x_3 , and t_3, t_4 are passing points of intervals (x_1, x_2) and (t_1, t_2) .

Further, with the use of the theorem of finite decrements the latter equation can be transformed to have the following statement:

$$-w S_{tr} \frac{\partial c(x, t)}{\partial x} \Big|_{\substack{t_3 \in (t_1, t_2) \\ x_4 \in (x_1, x_2)}} \Delta t \Delta x + S_{tr} \frac{\partial}{\partial x} \left(D_g(x) \frac{\partial}{\partial x} c(x, t) \right) \Big|_{\substack{t_4 \in (t_1, t_2) \\ x_5 \in (x_1, x_2)}} \Delta t \Delta x - \\ - \frac{V_{ai}}{\Delta x} \frac{\partial a(t)}{\partial t} \Big|_{t_5 \in (t_1, t_2)} \Delta t \Delta x = S_{tr} \frac{\partial c(x, t)}{\partial t} \Big|_{\substack{x_3 \in (x_1, x_2) \\ t_6 \in (t_1, t_2)}} \Delta x \Delta t.$$

After the restriction on $\Delta t \Delta x$ we obtain:

$$-w \frac{\partial c(x, t)}{\partial x} \Big|_{\substack{t_3 \in (t_1, t_2) \\ x_4 \in (x_1, x_2)}} + \frac{\partial}{\partial x} \left(D_g(x) \frac{\partial}{\partial x} c(x, t) \right) \Big|_{\substack{t_4 \in (t_1, t_2) \\ x_5 \in (x_1, x_2)}} - \\ - \frac{V_{ai}}{S_{tr} \Delta x} \frac{\partial a(t)}{\partial t} \Big|_{t_5 \in (t_1, t_2)} = \frac{\partial c(x, t)}{\partial t} \Big|_{\substack{x_3 \in (x_1, x_2) \\ t_6 \in (t_1, t_2)}}.$$

These considerations apply to any time intervals (x_1, x_2) and (t_1, t_2) . Passing to a limit of $x_1, x_2 \rightarrow x$ and $t_1, t_2 \rightarrow t$, we obtain a differential equation of nitrogen diffusion in gas-air mixture at a time interval $(n-1)t_c < t < (n-1/2)t_c$, $n = 1, 2, \dots$

$$-w \frac{\partial c(x, t)}{\partial x} + \frac{\partial}{\partial x} \left(D_g(x) \frac{\partial}{\partial x} c(x, t) \right) - \frac{V_{ai}}{S_{tr} \Delta x} \frac{\partial a_i(t)}{\partial t} = \frac{\partial c(x, t)}{\partial t}$$

or, introducing a symbol $\varepsilon_i = \frac{V_{tri}}{V_{ai} + V_{tri}}$, we obtain

$$\frac{\partial c(x,t)}{\partial t} + \frac{1-\varepsilon_i}{\varepsilon_i} \frac{\partial a_i(t)}{\partial t} = -w \frac{\partial c(x,t)}{\partial x} + \frac{\partial}{\partial x} \left(D_g(x) \frac{\partial c(x,t)}{\partial x} \right), \quad (1)$$

where the number i of adsorbent layer corresponds to the coordinate x_i , for example, in the solution of equation (1) with respective boundary conditions with the help of finite-difference method, i corresponds to the interval (x_i, x_{i+1}) of the spatial coordinate x . Within this interval the nitrogen concentration in i layer of adsorbent is constant, i.e. $a_i = \text{const}$.

A similar equation describes the process of diffusion during nitrogen desorption at a time interval $(n-1/2)t_c < t \leq nt_c$, $n = 1, 2, \dots$

Using the methodology of derivation of diffusion equation described in Step 1, equations of mathematical model of other processes are obtained.

2. Changes of nitrogen concentration in adsorbent:

– in integral form in i layer of adsorbent over a time interval (t_1, t_2)

$$V_{ai}[a_i(t_2) - a_i(t_1)] = S_{ai}\beta \int_{t_1}^{t_2} \left[a_i^* \left(\bar{c}_i, \bar{T}_{gi} \right) - \bar{c}_i(t) \right] dt, \quad i = 1, \dots, N;$$

– in differential form over a time interval $(n-1)t_c < t < (n-1/2)t_c$, $n = 1, 2, \dots$

$$V_{ai} \left(\frac{\partial a_i(t)}{\partial t} \right) = \beta S_{ai} (a_i^* (\bar{c}(t), \bar{T}_g(t)) - c_i(t)); \quad i = 1, \dots, N, \quad (2)$$

where $\bar{c}(t) = (c(x_i, t) + c(x_{i+1}, t))/2$, $\bar{T}_g(t) = (T_g(x_i, t) + T_g(x_{i+1}, t))/2$, $i = 1, 2, \dots, N$.

3. Heat propagation in gas-air mixture over the adsorbent's height:

– in integral form in an interval (x_1, x_2) over a time period (t_1, t_2)

$$c_p^g \rho_g W_g \int_{t_1}^{t_2} [T_g(x_1, t) - T_g(x_2, t)] dt + S_{tr} \int_{t_1}^{t_2} \left[(-\lambda(x_1) \frac{\partial T_g(x_1, t)}{\partial x}) - (-\lambda(x_2) \frac{\partial T_g(x_2, t)}{\partial x}) \right] dt + \\ + \alpha S_{ai} \int_{t_1}^{t_2} (T_{ai}(t) - \bar{T}_{gi}(t)) dt + c_p^g \rho_g S_{tr} \int_{x_1}^{x_2} [T_g(x, t_2) - T_g(x, t_1)] dx = 0;$$

– in differential form over a time period $(n-1)t_c < t < (n-1/2)t_c$, $n = 1, 2, \dots$

$$-c_p^g \rho_g w \frac{\partial T_g(x, t)}{\partial x} + \frac{\partial}{\partial x} \left(\lambda(x) \frac{\partial T_g(x, t)}{\partial x} \right) + \left(\frac{1-\varepsilon_i}{\varepsilon_i} \right) \alpha \sigma [T_{ai}(t) - \bar{T}_{gi}(t)] + \\ + c_p^g \rho_g \frac{\partial T_g(x, t)}{\partial t} = 0, \quad 0 < x < H, \quad (3)$$

where σ is specific area of adsorbent's transporting pores, m^2/m^3 .

A similar equation is used to describe the process of heat propagation in gas-air mixture during nitrogen desorption over a time interval $(n-1/2)t_c < t \leq nt_c$, $n = 1, 2, \dots$

4. Temperature changes in adsorbent:

– in integral form in i layer of adsorbent over a time interval (t_1, t_2)

$$- \alpha S_{ai} \int_{t_1}^{t_2} [T_{ai}(t) - \bar{T}_{gi}(t)] dt + h_{ad} [a_i(t_2) - a_i(t_1)] V_{ai} = c_p^a \rho_a V_{ai} [T_{ai}(t_2) - T_{ai}(t_1)],$$

– in differential form over a time interval $(n-1)t_c < t < (n-1/2)t_c$, $n = 1, 2, \dots$

$$c_p^a \rho_a \frac{\partial T_{ai}(t)}{\partial t} + \left(\frac{1-\varepsilon_i}{\varepsilon_i} \right) \alpha (T_{ai}(t) - \bar{T}_g(t)) - h_{ad} \frac{\partial a_i(t)}{\partial t} = 0. \quad (4)$$

A similar equation describes the process of heat propagation in adsorbent during nitrogen desorption at a time interval $(n-1/2)t_c < t \leq nt_c$, $n=1,2,\dots$ except that h_{des} is used instead of h_{ad} .

5. Changes in velocity of gas-air mixture over the height of adsorbent:

– in integral form in an interval (x_1, x_2) over a time period (t_1, t_2)

$$-S_{tr} \int_{t_1}^{t_2} [w(x_2, t) - w(x_1, t)] dt - V_{ai} [a_i(t_2) - a_i(t_1)] M_{N_2} / \rho_{N_2} = 0,$$

– in differential form over a time period $(n-1)t_c < t < (n-1/2)t_c$, $n=1,2,\dots$

$$-\frac{\partial w}{\partial x} - \frac{M_{N_2}}{\rho_{N_2}} \left(\frac{1-\varepsilon}{\varepsilon} \right) \frac{\partial a_i(t)}{\partial t} = 0. \quad (5)$$

A process of velocity change in gas-air mixture during nitrogen desorption over a time period $(n-1/2)t_c < t \leq nt_c$, $n=1,2,\dots$ can be similarly described.

The initial conditions for equations (1) – (5) are stated as following:

– as $t=0$

$$a_i(0) = 0, \quad c(x,0) = c_0, \quad T_{ai}(0) = T_{a0}, \quad T_g(x,0) = T_{g0}, \quad 0 \leq x \leq H; \quad (6)$$

– as $t=n \times t_c$, $n=1,2,\dots$:

$$a_i(t) = a_i^{des}(t_c), \quad c(x,t) = c^{des}(x,t_c), \quad T_{ai}(t) = T_{ai}^{des}(t_c), \quad (7)$$

$$T_g(x,t) = T_g^{des}(x,t_c), \quad 0 \leq x \leq H,$$

– for desorption process as $(n-1/2)t_c$, $n=1,2,\dots$:

$$a_i^{des}(t) = a_i(t_c/2), \quad c^{des}(x,t) = c(x,t_c/2), \quad T_a^{des}(x,t) = T_a(x,t_c/2),$$

$$T_g^{des}(x,t) = T_g(x,t_c/2), \quad 0 \leq x \leq H. \quad (7')$$

The boundary conditions for adsorption process at $(n-1)t_c \leq t \leq (n-1/2)t_c$, $n=1,2,\dots$ and desorption process at $(n-1/2)t_c < t \leq nt_c$, $n=1,2,\dots$ were assumed as following:

– for adsorption process as $x=0$

$$c^{ad}(0,t) = c_{in}, \quad T_g^{ad}(0,t) = T_g^{in}, \quad w(0,t) = w_{in}, \quad (8)$$

as $x=H$

$$\frac{\partial c(H,t)}{\partial x} = 0, \quad \frac{\partial T_g(H,t)}{\partial x} = 0, \quad \frac{\partial w(H,t)}{\partial x} = 0; \quad (9)$$

– for desorption process as $x=0$

$$\frac{\partial c(H,t)}{\partial x} = 0, \quad \frac{\partial T_g(H,t)}{\partial x} = 0, \quad \frac{\partial w(H,t)}{\partial x} = 0, \quad (8')$$

as $x=H$

$$c^{des}(H,t) = c(H,t_{ad}), \quad T_g^{des}(H,t) = T_g(H,t_{ad}), \quad w(H,t) = w(H,t_{ad}). \quad (9')$$

The coefficient D_g of nitrogen diffusion in gas phase was calculated by Fuller-Schettler-Giddings method [15] (see Table 1), and differential mole heat of adsorption h_{ad} and h_{des} was determined on the basis of thermal equation of the theory of micropore volumetric filling [8]. The equilibrium adsorption value a_i^* was calculated with the use Dubinin-Radushkevich equation [8, 9]. The saturation pressure P^* , the coefficient of heat exchange α , and the coefficient of mass transfer β were found according to recommendations given in works [16] and [17] respectively (see Table 1). The volume rate of flow was determined using the formula

$$W_{in} = W_{giv} / \left(1 - \theta \frac{P_{des}}{P_{ad}} \right), \quad (10)$$

where θ is a backwashing coefficient which characterizes a portion of oxygenated air flow that is returned for nitrogen desorption [1].

The formulae for calculating the coefficients of mathematical model equations are presented in Table 1.

Table 1

Formulae for model's coefficients calculation

$P^* = \exp \left(A - \frac{F}{(T_g - C)} \right) / 760;$	(11)
$v_i = \frac{M_i}{\rho_{cr,i} \exp(\varphi(T_{cr,i} - T_g))}, \quad i = N_2, O_2;$	(12)
$a_i^* = \frac{W_0}{22,4\bar{c}_i v_{N_2}} \exp \left(- \frac{BT_a^2}{(22,4\bar{c}_i \psi)^2} \left(\log \left(\frac{P^*}{22,4\bar{c}_i P} \right) \right)^2 \right);$	(13)
$h_{ad} = \gamma_{N_2} + E_0 \left[\left(\ln \left(\frac{a_i^*}{a_i} \right) \right)^{\frac{1}{n}} + \left(\frac{\varphi T_a}{n} \right) \left(\ln \left(\frac{a_i^*}{a_i} \right) \right)^{\frac{1}{n}-1} \right];$	(14)
$h_{des} = \gamma_{N_2} + E_0 \left[1 + \left(\ln \left(\frac{a_i^*}{a_i} \right) \right)^{\frac{1}{n}} + \left(\frac{\varphi T_a}{n} \right) \left(\ln \left(\frac{a_i^*}{a_i} \right) \right)^{\frac{1}{n}-1} \right];$	(15)
$D_g = \frac{10^{-7} T_g^{1,75} [(M_{N_2} + M_{O_2}) / (M_{N_2} M_{O_2})]^{1/2}}{P [(v_{N_2})^{1/3} + (v_{O_2})^{1/3}]^2};$	(16)
$\beta = 0,355 \frac{w}{\varepsilon \rho_a} \left(\frac{w \rho_g d_e}{\mu} \right)^{0,359} \left(\frac{\mu}{\rho_g D_g} \right)^{-0,667};$	(17)
$\alpha = \frac{0,24 \text{Re}_e^{0,83} \lambda}{d_e};$	(18)
$\rho(c) = \frac{(1 - 22,4c)32}{22,4} P;$	(19)
$\Delta P = 150 \frac{(1 - \varepsilon)^2 \eta w_0}{\varepsilon^3 d_e} x + 1,54 \frac{1 - \varepsilon}{\varepsilon^3} \frac{\rho_g w_0^2}{d_e}, \quad w_0 = w/S.$	(20)

In the presented formulae: $A, C, F, \psi, \gamma, \phi$ are nitrogen constants, B, n are zeolite constants, ρ_{cr} is critical density, and T_{cr} is critical temperature [15].

Algorithm of Numerical Solution of Equations of Air Oxygenation Model

The system of differential equations (1) – (5) is nonlinear since the coefficients a_i^* , $h_{ad}(a_i)$, $h_{des}(a_i)$ depend on current values of nitrogen concentration in gas phase c and adsorbent temperature T_a , respectively. To solve it, we have developed an iteration algorithm in the Matlab software environment implementing the method of finite elements [18, 19]. The algorithm scheme is presented in Fig. 4.

In the first block design parameters of the installation and regime variables of its functioning are set, as well as kinetic, physical and chemical constants that are included in coefficients of mathematical model equations (1) – (5), and tuning parameters of the algorithms of numerical solution of differential equations of mass and heat transfer.

The second block begins with the calculation of oxygenation process – adsorption: control variables bb and ab are assigned values «A» («A» stands for the calculation of adsorption process and «D» – for the calculation of desorption process) and «I» («I» means iteration cycle, «NI» – no iteration cycle), i.e. $bb := A$, $ab := I$. Also, initial approximations for equations (1) – (5) are given.

In block 3 the state variables of air oxygenation process are re-assigned depending on the number of iteration v .

In block 4 the calculations of coefficients of mathematical model (1) – (5) are successively performed (Table 1).

In block 5, using the method of finite elements, the values of $c^{(v)}(x_i, t_j)$; $a_i^{(v)}(t_j)$; $T_g^{(v)}(x_i, t_j)$; $T_{ai}^{(v)}(t_j)$, $w^{(v)}(x_i, t_j)$, $i = \overline{0, n}$ at the next iteration are computed.

In block 6 the iteration cycle is checked for the convergence conditions:

$$\left| \frac{g_{ij}^{(v+1)} - g_{ij}^{(v)}}{g_{ij}^{(v)}} \right| \leq \delta, \quad g_{ij} = (c_{ij}, a_j, T_{gij}, T_{aj}, w_{ij});$$

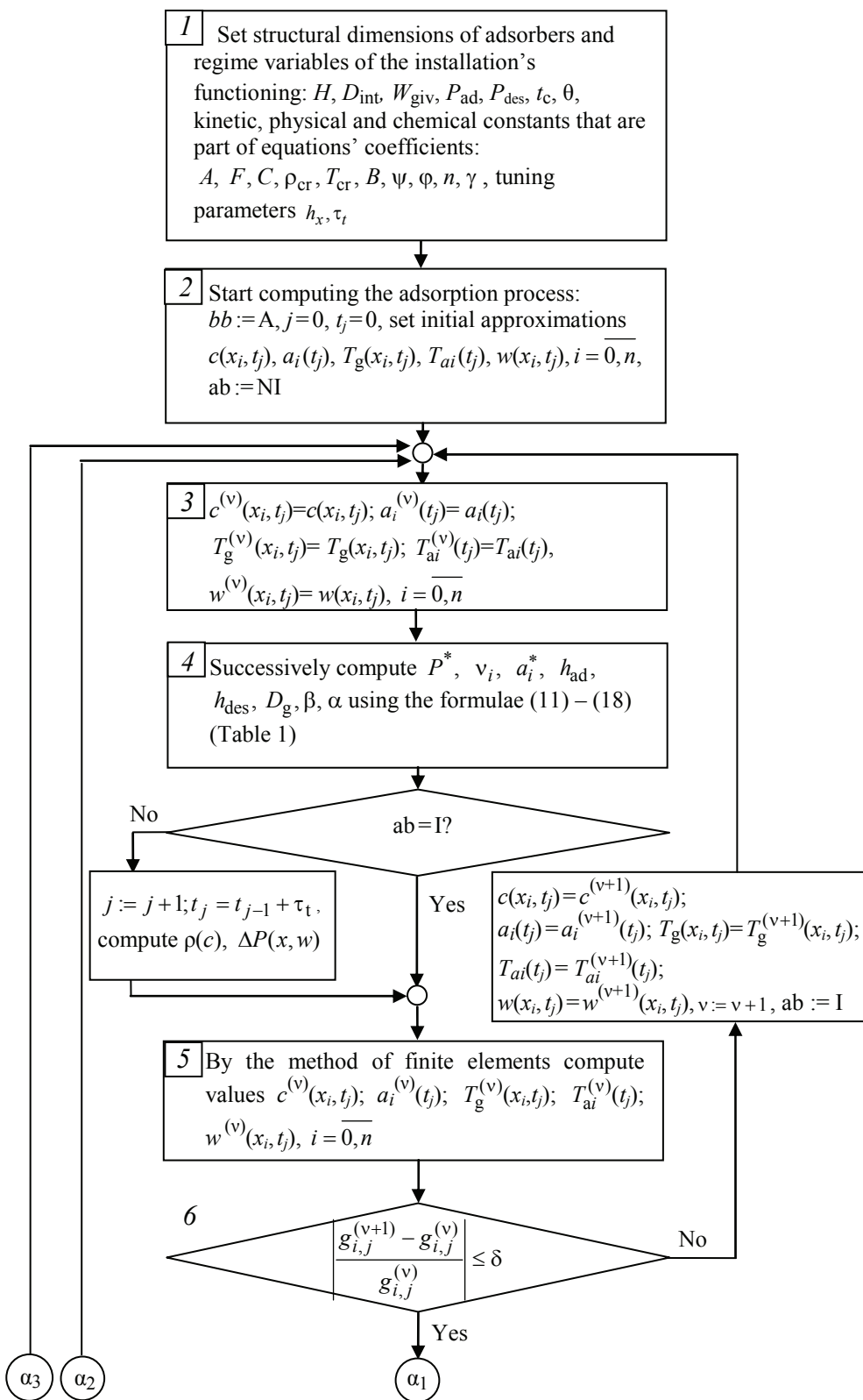
$$\left| \frac{c_{ij}^{(v+1)} - c_{ij}^{(v)}}{c_{ij}^{(v)}} \right| \leq \delta; \quad \left| \frac{a_j^{(v+1)} - a_j^{(v)}}{a_j^{(v)}} \right| \leq \delta; \quad \left| \frac{T_{gij}^{(v+1)} - T_{gij}^{(v)}}{T_{gij}^{(v)}} \right| \leq \delta;$$

$$\left| \frac{T_{aj}^{(v+1)} - T_{aj}^{(v)}}{T_{aj}^{(v)}} \right| \leq \delta; \quad \left| \frac{w_{ij}^{(v+1)} - w_{ij}^{(v)}}{w_{ij}^{(v)}} \right| \leq \delta.$$

Block 7 checks whether the end of calculation condition for the process of adsorption is fulfilled: $t_j = (N-1/2)t_c$? If this condition is fulfilled, the calculations for the desorption process are carried out (block 8, $bb := D$).

When a given number of cycles is performed $N = N_{giv}$ (block 9), the computation ends.

In block 10 the state variables of air oxygenation process are re-assigned depending on the number of iteration v .



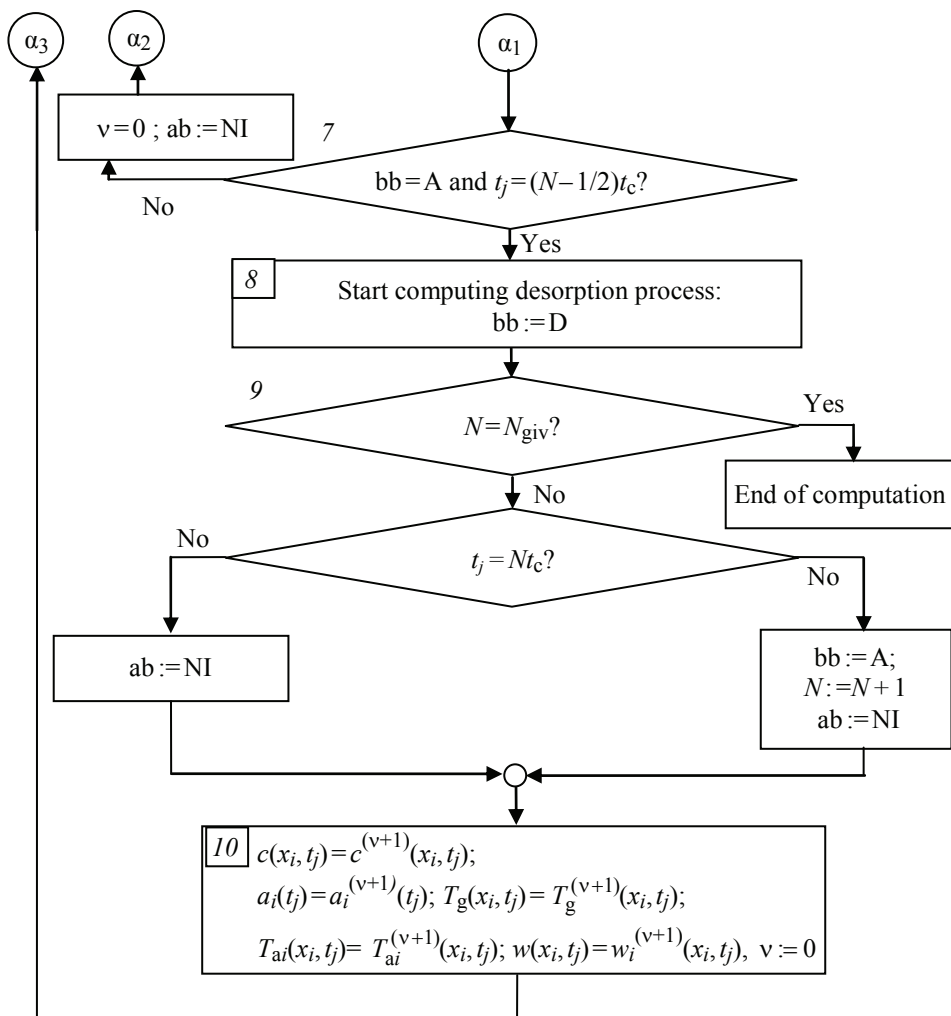


Fig. 4. Scheme of iteration algorithm for the solution of differential equations (1) – (5):
 I – iteration cycle; NI – no iteration cycle; A – adsorption process is calculated;
 D – desorption process is calculated

When modeling air oxygenation process, the characteristics of LiLSX [4] adsorbent were assumed to be the following (Table 2).

The model's adequacy was checked by comparing the values of oxygen concentration at the PSA unit's outlet as calculated according to the model (firm lines) and experimentally obtained (dash-and-dot lines), see Fig. 5.

The maximal disparity between the modeled and experimental values of oxygen concentration at the unit's outlet over a functioning cycle does not exceed 12 %.

Table 2

Characteristics of LiLSX adsorbent

Characteristic	Value
$E_0, \text{J}\cdot\text{mole}^{-1}$	16800
ε	0,394
B, K^{-2}	$1,28 \times 10^{-6}$
ψ	1
$W_0, \text{sm}^3\cdot\text{g}^{-1}$	0,195
$c_p^a, \text{J}\cdot(\text{kg}\cdot\text{K})^{-1}$	700
$\rho_a, \text{kg}\cdot\text{m}^{-3}$	660
d_e, m	2×10^{-4}

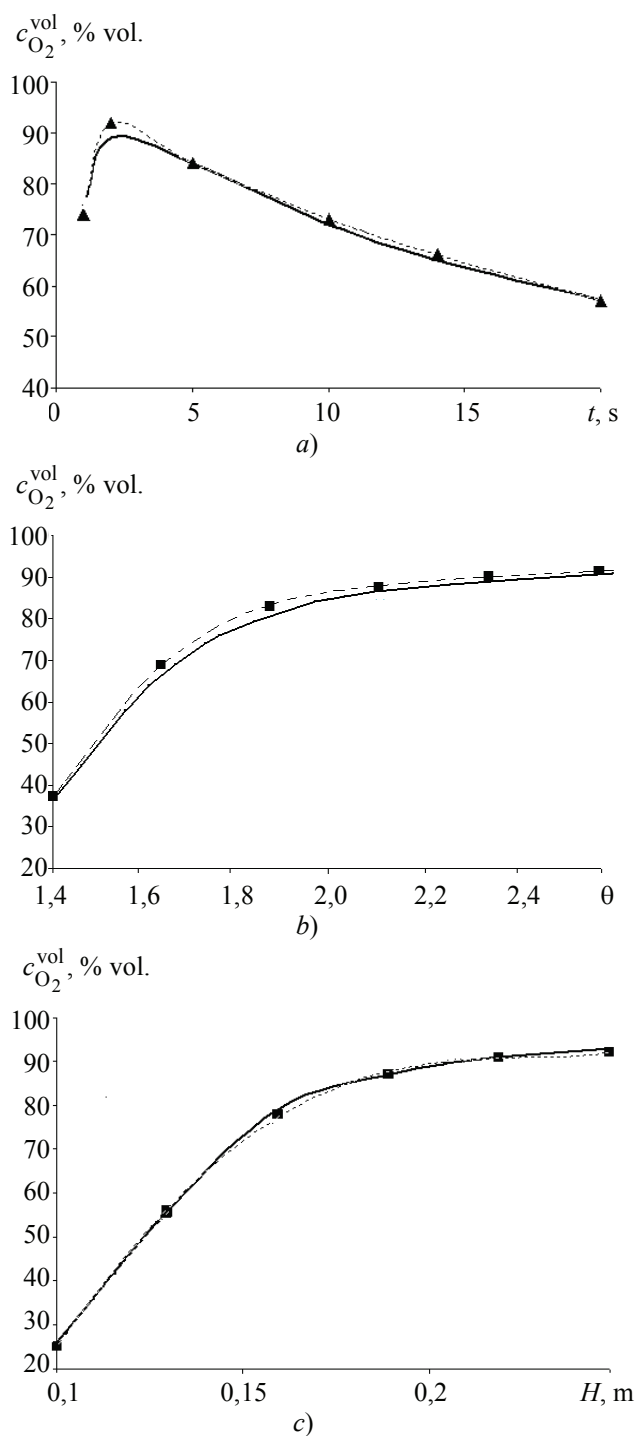


Fig. 5. Calculated and experimentally obtained dependencies between oxygen concentration and duration of cycle (a), backwashing coefficient (b), height of LiLSX adsorbent layer (c):

$$H = 0,25 \text{ m}; V_{\text{work}} = 0,25 \times 10^{-3} \text{ m}^3; W_{\text{in}} = 0,167 \times 10^{-3} \text{ m}^3/\text{s};$$

$$\theta = 2,5; D_e = 0,20 \text{ mm}; t_c = 5 \text{ s}$$

Fig. 6 presents the profiles of oxygen concentration in gas phase over the adsorbent's height as depending on time during adsorption (*a*) and desorption (*b*). Fig. 7 shows dependences between oxygen concentration in gas phase and aerodynamic resistance of adsorbent and the value of ratio of adsorbent layer's height to adsorber's diameter.

The analysis of graphs in Fig. 7 proves that the maximal oxygen concentration is reached when H/D_{int} values range from 4 to 6; when $H/D_{\text{int}} > 8$, the layer's resistance monotonically increases, which results in the reduction of P_{ad} and, subsequently, in the decrease of oxygen concentration at the unit's outlet.

Computing experiments have also established the fact that oxygen concentration at the outlet reaches its maximal value $c_{\text{O}_2}^{\text{vol}} = 91,1\%$ when the number of adsorption-desorption cycles is no less than $n_c = 18$.

Using the mathematical model of heat and mass transfer processes during air oxygenation the method and computer program for process design of the pressure swing adsorption unit have been developed. They allowed determining such design (adsorbent

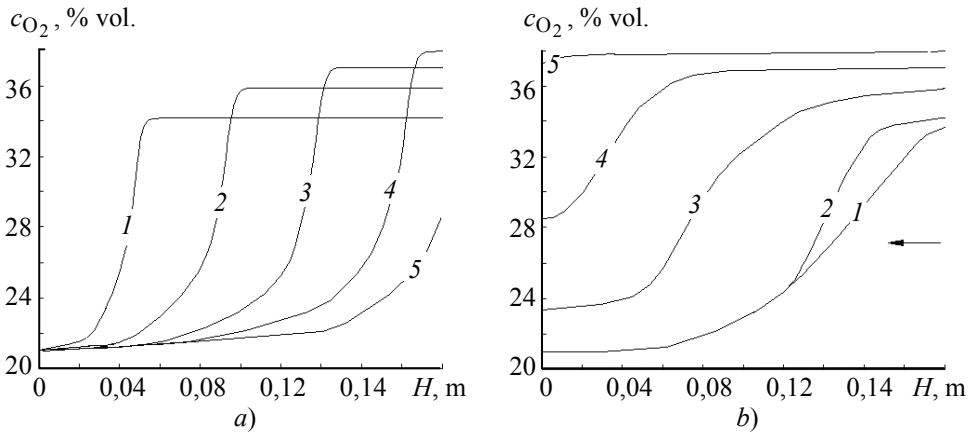


Fig. 6. Changes in oxygen concentration in gas phase in cycle 1:
a – during adsorption; *b* – during desorption;
 1 – $t = 0,2$; 2 – $t = 0,4$; 3 – $t = 0,6$; 4 – $t = 0,8$; 5 – $t = 1,0$

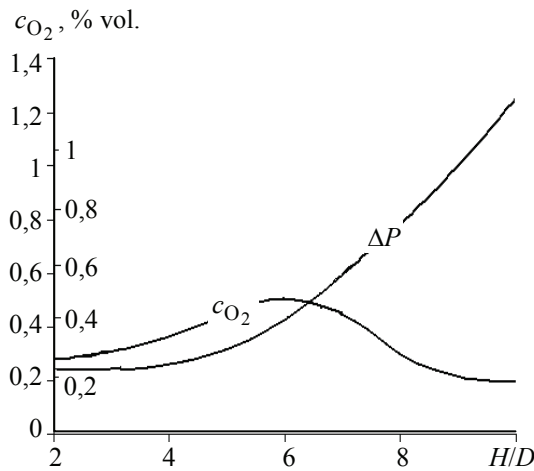


Fig. 7. Oxygen concentration and layer's aerodynamic resistance depending on the ratio of the height to adsorber's diameter:

$$V_{\text{work}} = 0,25 \times 10^{-3} \text{ m}^3, d_e = 0,2 \text{ mm}$$

layer's height, adsorber's diameter) and regime (controlling) variables of the unit (cycle duration, backwashing coefficient) that satisfy the given values for productivity $W_{giv}=0.05\times 10^{-3}$ m³/s and oxygen concentration $[c_{O_2}^{vol}]_{giv} \geq 90\%$.

The problem of optimal design (by capital costs criterion) of energy-saving unit for pressure swing adsorption with the productivity $W_{giv} = 0,05\times 10^{-3}$ m³/s and oxygen concentration $c_{O_2}^{vol} \sim 90\%$ has been formulated and solved. Design parameters for the two-adsorber unit with vacuum desorption, which can be implemented as a medical oxygen concentrator, have been determined: $H^* = 0,22$ m, $D_{int}^* = 0,035$ m; its regime variables should be $P_{ad}^* = 1,5\times 10^5$ Pa, $P_{des}^* = 0,5\times 10^5$ Pa, $\theta^* = 2,5$, $t_c^* = 1,6$ s, $G_{in}^* = 2,93\times 10^{-4}$ m³/s; and performance characteristics should be the following: capital costs $CC^* = 45,250$ roubles, mass $m^* = 0,5$ kg, and power consumption $N_{cons}^* = 76$ Wt.

CONCLUSION

Solving the problem of optimal design practical recommendations for the design of aircraft units for oxygen production and medical oxygen concentrators, with productivity ranges up to 10^{-3} m³/s and $0,08\times 10^{-3}$ m³/s respectively, have been developed. Block zeolite adsorbents of LiLSX zeolite type with $d_e \leq 0,5\times 10^{-3}$ m are recommended for implementation in adsorbers which comply with the following condition: $4 \leq H/D_{int} \leq 6$ when pressure scheme with vacuum desorption is realized ($P_{ad}/P_{des} \leq 3$). The application of these recommendations allows lowering unit mass by 25% and decreasing energy consumption by 20% as compared with existing analogues.

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Моделирование процесса обогащения воздуха кислородом путем поглощения азота в установке короткоциклового адсорбции

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Ключевые слова и фразы: адсорбция азота; математическая модель; медицинский концентратор кислорода; обогащение воздуха кислородом; технология короткоциклового адсорбции; цеолитовый адсорбент;

Аннотация: Разработаны математическая модель и алгоритм решения уравнений модели динамики обогащения воздуха кислородом в двухадсорберной установке короткоциклового адсорбции с вакуумной десорбцией, предназначенной для лечения и профилактики больных хроническими легочными заболеваниями. Методом математического моделирования исследованы массо- и теплообменные процессы при адсорбции азота из газовой смеси блочным цеолитовым адсорбентом.

Modellierung des Prozesses der Anreicherung der Luft vom Sauerstoff durch die Absorption des Stickstoffes in der Anlage der Kurzzyklusabsorption

Zusammenfassung: Es sind das mathematische Modell und den Algorithmus der Lösung der Gleichungen des Modells der Dynamik der Anreicherung der Luft vom Sauerstoff in der Anlage der Kurzzyklusabsorption mit der Vakuumdesorption, die für die Behandlung und die Vorbeugung der Kranken mit den chronischen Lungenerkrankungen vorherbestimmt sind, erarbeitet. Durch die Methode der mathematischen Modellierung sind die Massen- und Wärmeübertragungsprozesse bei der Absorption des Stickstoffes aus dem Gasluftgemisch vom Blockzeolithadsobens untersucht.

Modélage du processus de l'enrichissement de l'air par l'oxygène par la voie de l'absorption de l'azote dans une installation de l'absorption de cycle court

Résumé: Sont élaborés le modèle mathématique et l'algorithme de la solution des équations du modèle de la dynamique de l'enrichissement de l'air par l'oxygène dans une installation de deux sorbants de l'absorption de cycle court avec une désorption à vide destiné au traitement et à la prophylaxie des poitrinaires. Par la méthode de modélage mathématique sont étudiés les transferts de masse et de chaleur lors de l'absorption de l'azote à partir du mélange air-gaz par un absorbant zeolitic préfabriqué.

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