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 chronical 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\(^3\);
\(a^*\) – equilibrium adsorption value, mole/m\(^3\);
\(A\) – nitrogen constant;
\(B\) – coefficient of equations of micropore
volumetric filling theory, K\(^{-2}\);
\(C_p\) – heat capacity, J/(kg \cdot K);
\(C\) – nitrogen constant;
\(c\) – concentration in gas phase, mole/m\(^3\);
\(c_{O_2}\) – oxygen concentration in gas phase at the
unit’s outlet, m\(^3\)/m\(^3\), \% vol.;
\(D_{int}\) – internal diameter of adsorber, m;
\(D_g\) – diffusion coefficient in gas phase, m\(^2\)/s;
\(d_e\) – equivalent diameter of adsorbent’s
transporting pores, m;
\(E_0\) – characteristic adsorption energy, J/mole;
\(F\) – nitrogen constant;
\(h\) – thermal effect, J/mole;
\(h_x\) – coordinate pitch distance in finite elements
grid, m;
\(H\) – height of adsorbent layer, m;
\(m\) – mass, kg;
\(M\) – molar mass, kg/kmole;
\(N\) – number of grid cells;
\(N_{cons}\) – power consumption, Wt;
\(n\) – degree index in equations of micropore
volumetric filling theory;
\(n_c\) – number of adsorption-desorption cycles;
\(P\) – pressure, Pa;
\(P^*\) – saturation pressure, Pa;
\(R\) – universal gas constant, J/(mole \cdot K);
\(S\) – area, m\(^2\);
\(S_a\) – surface area of adsorbent’s transporting
pores, m\(^2\);
\(t\) – time, s;
\(T\) – temperature, K;
\(V\) – volume, m\(^3\);
\(V_{work}\) – adsorber’s working volume, m\(^3\);
\(W\) – volume flow rate, m\(^3\)/s;
\(W_0\) – maximum adsorption volume, sm\(^3\)/g;
\(w\) – speed of gas flow, m/s;
\(\alpha\) – heat exchange coefficient, Wt/(m\(^2\) \cdot K);
\(\beta\) – external mass transfer coefficient, m/s;
\(\gamma\) – condensation-evaporation heat, J/kg;
\(\delta\) – fixed precision of computation;
\(\varepsilon\) – volume fraction of transporting pores
(porosity coefficient);
\(\theta\) – backwashing coefficient;
\(\eta\) – kinematic viscosity of air, m\(^2\)/s;
\(\lambda\) – thermal conductivity coefficient, Wt/(m \cdot K);
μ – dynamic viscosity of air, Pa·s;
ν – molar volume, mole/m³;
ρ – density, kg/m³;
σ – specific surface area of adsorbent’s transporting pores, m²/m³;
τ – time pitch distance, s;
ψ – thermal coefficient of maximum adsorption;
ψ – affine property coefficient;

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

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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:

\[ P_{ad} \]
\[ P_{des} \]
\( \tau_c/2 \)
\( \tau_c \)
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 \( d_e \leq 0.5 \times 10^{-3} \text{ m} \) in equivalent diameter (adsorption volume limit is \( 0.195 \text{ sm}^3/\text{kg}^{-1} \) 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 \( \beta \) and value \( a^*_W(c, T_g) \) 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 \( T_{al} \) depend on time, i.e. \( a_i = a_i(t), \ T_{al} = T_{al}(t), \ i = 1, N \); 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.

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]:

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

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:

\[
-W_g \frac{\left[ c(x_2, t) - c(x_1, t) \right]}{\Delta x} \bigg|_{t_3 \in (t_1, t_2)} \Delta t \Delta x + S_{tr} \frac{\partial}{\partial x} \left( D_g(x) \frac{\partial}{\partial x} c(x, t) \right) \bigg|_{t_4 \in (t_1, t_2)} \Delta t \Delta x \\
\times \Delta t \Delta x - \frac{V_{ai} \left[ a_i(t_2) - a_i(t_1) \right]}{\Delta t} \bigg|_{t_5 \in (t_1, t_2)} \Delta t \Delta x = S_{tr} \frac{\partial c(x, t)}{\partial t} \bigg|_{t_6 \in (t_1, t_2)} \Delta t \Delta t,
\]

where \(\Delta x = (x_2 - x_1)\), \(x_3\), and \(t_3, t_4, t_5, t_6\) 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:

\[
-w \frac{\partial c(x, t)}{\partial x} \bigg|_{t_3 \in (t_1, t_2)} \frac{\partial^2 c(x, t)}{\partial x^2} \bigg|_{x_4 \in (x_1, x_2)} \Delta t \Delta x + S_{tr} \frac{\partial}{\partial x} \left( D_g(x) \frac{\partial}{\partial x} c(x, t) \right) \bigg|_{t_4 \in (t_1, t_2)} \Delta t \Delta x - \\
-V_{ai} \frac{\partial c(t)}{\partial t} \bigg|_{t_5 \in (t_1, t_2)} \Delta t \Delta t = S_{tr} \frac{\partial c(x, t)}{\partial t} \bigg|_{t_6 \in (t_1, t_2)} \Delta t \Delta t,
\]

After the restriction on \(\Delta t \Delta x\) we obtain:

\[
-w \frac{\partial c(x, t)}{\partial x} \bigg|_{t_3 \in (t_1, t_2)} \frac{\partial^2 c(x, t)}{\partial x^2} \bigg|_{x_4 \in (x_1, x_2)} + \frac{\partial}{\partial x} \left( D_g(x) \frac{\partial}{\partial x} c(x, t) \right) \bigg|_{t_4 \in (t_1, t_2)} \frac{\partial c(x, t)}{\partial t} \bigg|_{t_5 \in (t_1, t_2)} - \\
-V_{ai} \frac{\partial c(t)}{\partial t} \bigg|_{t_5 \in (t_1, t_2)} \Delta t \Delta t = S_{tr} \frac{\partial c(x, t)}{\partial t} \bigg|_{t_6 \in (t_1, t_2)} \Delta t \Delta t.
\]

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 \((n-1)t_e < t < (n-1/2)t_e, n = 1, 2, \ldots\)

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

or, introducing a symbol \(\varepsilon_i = \frac{V_{ai}}{S_{tr} \varepsilon_t + V_{ti}}\), we obtain
\[
\frac{\partial c(x,t)}{\partial t} + \frac{1}{v_i} \frac{\partial a_i(t)}{\partial t} = -w \frac{\partial c(x,t)}{\partial x} + \frac{\partial}{\partial x}\left(D_g(x) \frac{\partial}{\partial x} c(x,t)\right),
\]

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 \((n-1/2)t_c < t \leq nt_c\), \(n = 1, 2, \ldots\) 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 \((t_1, t_2)\)

\[V_{ai}[a_i(t_2) - a_i(t_1)] = S_{ai} \int_{t_1}^{t_2} a_i^{*} (\bar{c}(t), \bar{g}(t)) - c_i(t) \, dt, \quad i = 1, \ldots, N;\]
- in differential form over a time interval \((n-1)t_c < t < (n-1/2)t_c\), \(n = 1, 2, \ldots\)

\[V_{ai}\left(\frac{\partial a_i(t)}{\partial t}\right) = \beta S_{ai} (a_i^{*} (\bar{c}(t), \bar{g}(t)) - c_i(t)); \quad i = 1, \ldots, N,\]

where \(\bar{c}(t) = (c(x_1, t) + c(x_{i+1}, t))/2\), \(\bar{g}(t) = (g(x_1, t) + g(x_{i+1}, t))/2\), \(i = 1, 2, \ldots, N,\)

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 \rho_g W_g \int_{t_1}^{t_2} \left[T_g(x_1, t) - T_g(x_2, t)\right] dt + S_{tr} \sum_{i=1}^{2} \left[\frac{\partial T_g(x_1, t)}{\partial x} - \frac{\partial T_g(x_2, t)}{\partial x}\right] \right] dt +
+ \alpha S_{ai} \int_{t_1}^{t_2} (T_{ai}(t) - \bar{g}(t)) dt + c_p \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 \((n-1)t_c < t < (n-1/2)t_c\), \(n = 1, 2, \ldots\)

\[-c_p \rho_g v \frac{\partial T_g(x,t)}{\partial x} + \frac{\partial}{\partial x}\left(\lambda(x) \frac{\partial T_g(x,t)}{\partial x}\right) + \left(1 - \frac{1}{v_i}\right) \alpha \sigma [T_{ai}(t) - \bar{g}(t)] +
+ c_p \rho_g \frac{\partial T_g(x,t)}{\partial t} = 0, \quad 0 < x < H ,\]

where \(\sigma\) 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 \((n-1/2)t_c < t \leq nt_c\), \(n = 1, 2, \ldots\)

4. Temperature changes in adsorbent:
- in integral form in \(i\) layer of adsorbent over a time interval \((t_1, t_2)\)

\[-\alpha S_{ai} \int_{t_1}^{t_2} [T_{ai}(t) - \bar{g}(t)] dt + h_{ad}[a_i(t_2) - a_i(t_1)] V_{ai} = c_p \rho_a V_{ai} [T_{ai}(t_2) - T_{ai}(t_1)],\]
- in differential form over a time interval \((n-1)t_c < t < (n-1/2)t_c\), \(n = 1, 2, \ldots\)

\[c_p \rho_a \frac{\partial T_{ai}(t)}{\partial t} + \left(1 - \frac{1}{v_i}\right) \alpha (T_{ai}(t) - \bar{g}(t)) - h_{ad} \frac{\partial a_i(t)}{\partial t} = 0.\]
A similar equation describes the process of heat propagation in adsorbent during nitrogen desorption at a time interval \( (n-1/2)\tau_c < t \leq n\tau_c, \ n = 1, 2, \ldots \) except that \( h_{\text{des}} \) is used instead of \( h_{\text{ad}} \).

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 \((t_1, t_2)\)
     \[ -S_w \int_{t_1}^{t_2} [w(x_2, t) - w(x_1, t)] dt - V_w [a_i(t_2) - a_i(t_1)] M_{N_2}/\rho_{N_2} = 0, \]
   – in differential form over a time period \((n-1)\tau_c < t < (n-1/2)\tau_c, \ n = 1, 2, \ldots \)
     \[ -\frac{\partial w}{\partial x} - \frac{M_{N_2}}{\rho_{N_2}} \left(\frac{1 - \varepsilon}{\varepsilon}\right) \frac{\partial a_i(t)}{\partial t} = 0. \] (5)

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

The initial conditions for equations (1) – (5) are stated as following:
– as \( t = 0 \)
   \[ a_i(0) = 0, \ c(x,0) = c_0, \ T_{\text{ad}}(0) = T_{\text{ad}0}, \ T_g(x,0) = T_{\text{g0}}, \ 0 \leq x \leq H; \] (6)
– as \( t = n\tau_c, \ n = 1, 2, \ldots \)
   \[ a_i(t) = a_i^\text{des}(t_c), \ c(x,t) = c^\text{des}(x, t_c), \ T_{\text{ad}}(t) = T_{\text{ad}^\text{des}}(t_c), \]
   \[ T_g(x,t) = T_g^\text{des}(x, t_c), \ 0 \leq x \leq H, \] (7)
– for desorption process as \((n-1/2)\tau_c, \ n = 1, 2, \ldots:\)
   \[ a_i^\text{des}(t) = a_i(t_c/2), \ c^\text{des}(x,t) = c(x, t_c/2), \ T_{\text{ad}^\text{des}}(x,t) = T_{\text{a}}(x, t_c/2), \]
   \[ T_g^\text{des}(x,t) = T_g(x, t_c/2), \ 0 \leq x \leq H. \] (7')

The boundary conditions for adsorption process at \((n-1)\tau_c < t \leq (n-1/2)\tau_c, \ n = 1, 2, \ldots\) and desorption process at \((n-1/2)\tau_c < t \leq n\tau_c, \ n = 1, 2, \ldots\) were assumed as following:
– for adsorption process as \( x = 0 \)
   \[ c^\text{ad}(0,t) = c_{\text{in}}, \ T_{g^\text{ad}}(0,t) = T_{g^\text{in}}, \ w(0,t) = w_{\text{in}}, \] (8)
   as \( x = H \)
   \[ \frac{\partial c(H,t)}{\partial x} = 0, \ \frac{\partial T_g(H,t)}{\partial x} = 0, \ \frac{\partial w(H,t)}{\partial x} = 0; \] (9)
– for desorption process as \( x = 0 \)
   \[ \frac{\partial c(H,t)}{\partial x} = 0, \ \frac{\partial T_g(H,t)}{\partial x} = 0, \ \frac{\partial w(H,t)}{\partial x} = 0, \] (8')
   as \( x = H \)
   \[ c^\text{des}(H,t) = c(H, t_{\text{ad}}), \ T_{g^\text{des}}(H,t) = T_g(H, t_{\text{ad}}), \ w(H,t) = w(H, t_{\text{ad}}). \] (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 $\alpha$, and the coefficient of mass transfer $\beta$ 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

$$W_{in} = W_{giv} \left[ 1 - \theta \frac{P_{des}}{P_{ad}} \right],$$

where $\theta$ 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**

$$P^* = \exp \left( A - \frac{F}{(T_g - C)} \right) / 760;$$

$$v_i = \frac{M_i}{\rho_{cr,i} \exp(\Phi(T_{cr,i} - T_g))}, \quad i = N_2, O_2;$$

$$a_i^* = \frac{W_0}{22.4c_i N_{2}} \left[ \log \left( \frac{P^*}{22.4c_i P} \right) \right]^{1/2};$$

$$h_{ad} = \gamma_{N_2} + E_0 \left[ \ln \left( \frac{a_i^*}{a_i} \right) \right] \frac{1}{n} + \left( \frac{\Phi T_a}{n} \right) \left( \ln \left( \frac{a_i^*}{a_i} \right) \right) \frac{1}{n} - 1;$$

$$h_{des} = \gamma_{N_2} + E_0 \left[ 1 + \ln \left( \frac{a_i^*}{a_i} \right) \right] \frac{1}{n} + \left( \frac{\Phi T_a}{n} \right) \left( \ln \left( \frac{a_i^*}{a_i} \right) \right) \frac{1}{n} - 1;$$

$$D_g = \frac{10^{-7} T_g^{1.75 \left[ (M_{N_2} + M_{O_2}) / (M_{N_2} M_{O_2}) \right]^{1/2}}}{P \left( v_{N_2}^{1/3} + v_{O_2}^{1/3} \right)^2};$$

$$\beta = 0.355 \frac{w}{\rho_a} \left( \frac{w_p g d_e}{\mu} \right)^{0.359} \left( \frac{\mu}{\rho_g D_g} \right)^{-0.667};$$

$$\alpha = 0.24 \frac{Re_s}{d_e^{0.83}} \lambda;$$

$$\rho(c) = (1 - 22.4c) \frac{32}{22.4};$$

$$\Delta P = 150 \frac{(1 - e)^2 \eta w_0}{e^3 d_e} x + 1.54 \frac{1 - e \rho_g w_0^2}{e^3 d_e}, \quad w_0 = w/S. $$
In the presented formulae: $A, C, F, \psi, \gamma, \varphi$ are nitrogen constants, $B, n$ are zeolite constants, $\rho_{cr}$ 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 $\nu$.

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 $c^{(v)}(x_i, t_j); a_i^{(v)}(t_j); T_g^{(v)}(x_i, t_j); T_a^{(v)}(t_j), w^{(v)}(x_i, t_j), i = 0, n$ at the next iteration are computed.

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

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

$$
\left| \frac{c^{(v+1)}_{ij} - c^{(v)}_{ij}}{c^{(v)}_{ij}} \right| \leq \delta; \quad \left| \frac{a^{(v+1)}_{ij} - a^{(v)}_{ij}}{a^{(v)}_{ij}} \right| \leq \delta; \quad \left| \frac{T^{(v+1)}_{gij} - T^{(v)}_{gij}}{T^{(v)}_{gij}} \right| \leq \delta;
$$

$$
\left| \frac{T^{(v+1)}_{a_j} - T^{(v)}_{a_j}}{T^{(v)}_{a_j}} \right| \leq \delta; \quad \left| \frac{w^{(v+1)}_{ij} - w^{(v)}_{ij}}{w^{(v)}_{ij}} \right| \leq \delta.
$$

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 $\nu$. 

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Set structural dimensions of adsorbers and regime variables of the installation’s functioning: \( H, D_{\text{int}}, W_{\text{giv}}, P_{\text{ad}}, P_{\text{des}}, \theta, \) kinetic, physical and chemical constants that are part of equations’ coefficients: \( A, F, C, \rho_{\text{cr}}, T_{\text{cr}}, B, \psi, \varphi, n, \gamma, \) tuning parameters \( h_x, \tau_t \)

Start computing the adsorption process:

\[
\begin{align*}
&\text{ab} := A, j = 0, t = 0, \text{set initial approximations } \\
&c(x_i, t_j), a_i(t_j), T_g(x_i, t_j), T_{\text{ad}}(t_j), w(x_i, t_j), i = 0, n, \\
&\text{ab} := \text{NI}
\end{align*}
\]

1. Set structural dimensions of adsorbers and regime variables of the installation’s functioning:
2. Start computing the adsorption process:
3. Successively compute \( P^*, \nu_j, a^*, h_{\text{ad}}, h_{\text{des}}, D_g, \beta, \alpha \) using the formulae (11) – (18) (Table 1)
4. By the method of finite elements compute values \( c^{(v)}(x_i, t_j); a_i^{(v)}(t_j); T_{g}^{(v)}(x_i, t_j); T_{\text{ad}}^{(v)}(t_j); \)
5. \( w^{(v)}(x_i, t_j), i = 0, n \)
6. \[
\frac{|g_{i,j}^{(v+1)} - g_{i,j}^{(v)}|}{g_{i,j}^{(v)}} \leq \delta
\]
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

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(E_0), J-mole(^{-1})</td>
<td>16800</td>
</tr>
<tr>
<td>(\varepsilon)</td>
<td>0.394</td>
</tr>
<tr>
<td>(B), K(^{-2})</td>
<td>1.28×10(^{-6})</td>
</tr>
<tr>
<td>(\Psi)</td>
<td>1</td>
</tr>
<tr>
<td>(W_0), sm(^3)·g(^{-1})</td>
<td>0.195</td>
</tr>
<tr>
<td>(c_p^a), J·(kg·K(^{-1}))</td>
<td>700</td>
</tr>
<tr>
<td>(\rho_a), kg·m(^{-3})</td>
<td>660</td>
</tr>
<tr>
<td>(d_e), m</td>
<td>2×10(^{-4})</td>
</tr>
</tbody>
</table>
Fig. 5. Calculated and experimentally obtained dependencies between oxygen concentration and duration of cycle (a), backwashing coefficient (b), height of LiLSX adsorbent layer (c):

\[ H = 0.25 \text{ m}; \ V_{\text{work}} = 0.25 \times 10^{-3} \text{ m}^3; \ W_{\text{in}} = 0.167 \times 10^{-3} \text{ m}^3/\text{s}; \]

\[ \theta = 2.5; \ D_{\text{c}} = 0.20 \text{ mm}; \ t_{\text{c}} = 5 \text{ s} \]
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 $H/D_{int}>8$, 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 $c_{O_2}^{vol} = 91.1\%$ 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 volum.\%, $c_{O_2}$ vol.\%)

![Graph 6](image)

**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 – $t = 1.0$

![Graph 7](image)

**Fig. 7.** Oxygen concentration and layer’s aerodynamic resistance depending on the ratio of the height to adsorber’s diameter: 
$V_{work} = 0.25 \times 10^{-3} \text{ m}^3$, $d_c = 0.2 \text{ mm}$
layer’s height, adsorber’s diameter) and regime (controlling) variables of the unit (cycle duration, backwashing coefficient) that satisfy the given values for productivity $W_{giv} = 0.05\times10^{-3} \text{ m}^3/\text{s}$ and oxygen concentration $c_{O_2}^{vol} \geq 90\%$.

The problem of optimal design (by capital costs criterion) of energy-saving unit for pressure swing adsorption with the productivity $W = 0.05\times10^{-3} \text{ m}^3/\text{s}$ and oxygen concentration $c_{O_2}^{vol} \geq 90\%$ 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: $H^* = 0.22 \text{ m}$, $D^*_i = 0.035 \text{ m}$; its regime variables should be $P^*_{ad} = 1.5\times10^5 \text{ Pa}$, $P^*_{des} = 0.5\times10^5 \text{ Pa}$, $\theta^* = 2.5$, $t^*_c = 1.6 \text{ s}$, $G^*_m = 2.93\times10^{-4} \text{ m}^3/\text{s}$; and performance characteristics should be the following: capital costs $C^*_C = 45,250 \text{ roubles}$, mass $m^* = 0.5 \text{ kg}$, and power consumption $N^*_c = 76 \text{ Wt}$.

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 $10^{-3} \text{ m}^3/\text{s}$ and $0.08\times10^{-3} \text{ m}^3/\text{s}$ respectively, have been developed. Block zeolite adsorbents of LiLSX zeolite type with $d_c \leq 0.5\times10^{-3} \text{ m}$ are recommended for implementation in adsorbers which comply with the following condition: $4 \leq H/D_i \leq 6$ 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 короткоцикловой адсорбции

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

Аннотация: Разработаны математическая модель и алгоритм решения уравнений модели динамики обогащения воздуха кислородом в двухадсорберной установке короткоцикловой 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 газовоздушной смеси блочным цеолитовым адсорбентом.
Modellierung des Prozesses der Anreicherung der Luft vom Sauerstoff durch die Absorption des Stickstoffs in der Anlage der Kurzyzyklausorption


Modélage du processus de l'enrichissement de l’air par l’oxigène par la voie de l’absorption de l’azote dans une installation de l’aborption 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’aborption 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 zeolitique préfabriqué.


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