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A Numerical Study of Heat and Mass Exchange Processes in Swing Adsorption Device for Oxygen-Enriched Air

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Abstract

Using the developed mathematical model of the dynamics of cyclic adsorption processes for the separation of gas mixtures, numerical studies of heat and mass transfer processes in the PSA device for oxygen-enriched air have been carried out. Various programs have been studied to change the degree of opening of the inlet and outlet valves of the PSA device from the point of view of ensuring the maximum degree of oxygen concentration, a given value of the purity of the production gas and the permissible gas flow rate in the "front" layer of the adsorbent, at which the costly granular adsorbent is saved from destruction.

Keywords

Oxygen-enriched air; pressure swing adsorption; mathematical modeling; computational experiment; valve opening degree.

Introduction

One of the most effective and universal processes for purification and separation of gaseous media is cyclic adsorption processes carried out in pressure swing adsorption (**PSA**) devicess with a different number of adsorbers, receivers, valves and a complex process scheme. Various heat and mass transfer processes occur in adsorbers (more precisely, the adsorbent layer) (diffusion of the adsorbent in the gas mixture stream, mass transfer of the adsorbent and heat transfer between the gas phase and the adsorbent, adsorption of the adsorbent from the gas phase on the surface and in the micropores of the adsorbent granules with the release of heat and desorption adsorbate from micropores and from the surface of adsorbent granules into the gas phase with heat absorption) [1–8].

A distinctive feature of modern pressure swing adsorption processes and devices is the great complexity of the internal relationships of their parameters and characteristics, multi-stage processes (stages of adsorption and desorption of an adsorbent carried out under cyclically varying pressure; stages of drying and cooling of adsorbents, i.e. stages that mutually influence one another), the difference in energy costs for carrying out the stages of the process. The successful implementation of pressure swing adsorption processes and devices in industry depends, in particular, on improving existing processes, engineering methods for calculating the equilibrium of adsorbent-adsorbate systems, kinetics in an individual adsorbent grain and the dynamics of the adsorbent macrolayer, design solutions and methods for optimizing cyclic adsorption processes. As a result, an important link in the development of cyclic adsorption processes at the design stage is the selection of optimal options for the design of processes, the modes of various stages of the pressure swing adsorption process for specific operating conditions when separating gas mixtures [9–12].

When designing / calculating PSA devices, they often use so-called undefined ("inaccurate") information on physicochemical parameters (for example, temperature, pressure, environmental composition, kinetic parameters of heat and mass transfer processes, etc.), which indirectly has a noticeable effect on the quality of functioning of cyclic adsorption processes.

Another problem of the effective functioning of the PSA devices is the high gas flow rate in the frontal layer of the adsorbent, which leads to abrasion and destruction of the adsorbent granules [13–15]. It was shown in [16] that "careful" (stepwise opening of the intake valve) allows limiting the flow velocity in the frontal layer of the adsorbent, the maximum permissible value of which should not exceed ~ 0.2 m/s.

The aim of this research is a numerical study of heat and mass transfer processes in a PSA device for air-enriched oxygen and the influence of uncertain physicochemical parameters of cyclic adsorption processes on the efficiency of a PSA device, as well as a law (program) for changing the degree of inlet opening valves of the PSA device in time, providing the maximum degree of oxygen concentration, the specified purity of the production gas and the productivity of the installation, as well as the resource cutting of granular adsorbent.

The numerical study of heat and mass transfer processes and their influence on technological performance indicators of pressure swing adsorption processes

The technological process of oxygen concentration by adsorption separation of air is carried out in a two-adsorption PSA device with granular adsorbent – synthetic zeolite NaX [1–4, 17]. Input variables in PSA devices include raw material load G^{in} – flow rate of the initial gas-air mixture (atmospheric air); vector of controls $u=\{P^{\text{in}}, t_{\text{ads}}, \theta\}$; P^{in} – compressor outlet pressure; t_{ads} – adsorption stage duration (half cycle, $t_{\text{ads}}=t_{\text{des}}$); θ – backflow coefficient; uncertain parameters: temperature T_{g}^{in}; pressure P_1^{out} and component-wise composition y^{in} of the initial air-gas mixture fed to adsorbers for separation. Design parameters include the inner diameter of the adsorber D_{A}, absorber layer length L, adsorbent granule diameter d_{gr}. The output variables are the degree of oxygen extraction η, concentration y_1^{out} of production oxygen and related substances, performance Q of the PSA device.

A mathematical model of the dynamics of the cyclic adsorption process for air-enriched oxygen is given in [18, 19]. It includes the following equations:

1) component-wise material balance of components (O_2, N_2) in the gas phase flow, taking into account longitudinal mixing in the adsorbent layer (nonlinear partial differential equation of parabolic type);

2) kinetics of adsorption – desorption (nonlinear differential equation in ordinary derivatives);

3) heat distribution in the gas and solid phases, taking into account the convective component and thermal conductivity (nonlinear partial differential equations of parabolic type);

4) changes in the flow rate of the gas-air mixture and the pressure of the gas mixture (Ergun's differential equation in ordinary derivatives) along the height of the adsorbent.

To solve the equations of the mathematical model with the corresponding initial and boundary conditions, we used the direct method in the Matlab software environment [20].

A mathematical model of the dynamics of the cyclic process of adsorption concentration was used for the numerical study of heat and mass transfer processes and the influence of uncertain parameters on the output coordinates and technological performance indicators of the two-adsorption PSA device.

The source data for the computational experiments are presented in Table 1.

Fig. 1 shows the correlation graphs of oxygen concentration y_1^{out} in the production flow and duration $t_{\text{ads}}=t_{\text{c}}/2$ of adsorption-desorption half cycle for different values of pressure P^{in} at the compressor outlet and pressure $P_{\text{ads}}^{\text{in}}$ at the adsorption stage and temperature T_{g}^{in} of the environmental concentration of production oxygen and the PSA device performance.

From the analysis of the graphs it follows that with an increase in pressure P^{in} at the compressor outlet and, accordingly, the pressure at the adsorption stage, oxygen concentration y_1^{out} in the production flow and the PSA device performance increase. With an increase of P^{in} from $2\cdot10^5$ to $6\cdot10^5$ Pa, the gas-air flow rate in the adsorber increases, as a result of which the time of occurrence of an oxygen-enriched air flow at the outlet of the adsorber decreases (if $T_{\text{g}}^{\text{in}}=303$ K, $P^{\text{in}}=$ $=2\cdot10^5$ Pa, for $t_{\text{ads}}=3.5$ s, Fig. 1*a*, curve *3*; if $P^{\text{in}}=6\cdot10^5$ Pa, for $t_{\text{ads}}=0{,}5$ s, Fig. 1*e*, curve *3*).

Especially noticeable is an increase in the concentration and performance of the PSA device at elevated ambient temperature $T_{\text{g}}^{\text{in}}=303$ K (Fig. 1*a*, *b*, *e*, *f*, curve *3*), when the equilibrium nitrogen concentration and the amount of adsorbed nitrogen at the adsorption stage decrease.

Table 1

Source data for computational experiments

Source data	Nominal (working) values
The composition of the gas mixture i	1 – O_2; 2 – N_2; 3 – Ar
Zeolite adsorbent	NaX
Adsorption limit W_0, sm^3/g	0.17
Parameter B of the Dubinin equation, $\times 10^{-6}$ 1/K^2	6.55
Design parameters	
The number of adsorbents in the PSA device	2
Adsorbent inner diameter D_A, m	0.04
Adsorbent layer length L, m	0.2
Adsorbent granule diameter d_{gr}, mm	1.6
Receiver volume V_R, l	2

Variables	Range of variation	Nominal values
Load		
Flow capacity of input and output valves K_V, l/min	–	15
Compressor capacity G_C, l/min	1–50	10
Controls		
Adsorption stage duration t_{ads} (Adsorption-desorption half cycle), s	0.5–20	5
Compressor outlet pressure $P^{in} \times 10^{-5}$, Pa	2–6	4
Backflow coefficient θ, RU	1.0–2.4	1.7
Valve opening degree ψ_λ^j, RU	0–1	1
Uncertain parameters		
Component concentration in the initial mixture $y^{in} = y_{env}$	19.8–21.3; 78.2; 0.5–2.0	20.8; 78.2; 1.0
Initial mixture temperature $T_g^{in} = T_{env}$, K	243–303	293
Outlet device pressure $P_1^{out} = B_{env}$, $\times 10^{-5}$, Pa	0.25–1.0	1

With an increase of P^{in} from $2 \cdot 10^5$ to $6 \cdot 10^5$ Pa there is an increase in maximum concentration y_1^{out} of production oxygen from от 61 to 87 % vol. (Fig. 1*a*, *e*, curves *3*). An increase in y_1^{out} along with a decrease in θ and an increase in P^{in} provides an increase in the performance Q of the PSA device in oxygen enriched air (curves *3*, Fig. 1*b*, *d*, *f*). For example, at ambient temperature $T_g^{in} = 243$ K, $t_{ads} = 10$ s, the device performance with increasing pressure P^{in} increases from 0.21 (curve *1*, Fig. 1*b*) to 2.9 l/min (curve *1*, Fig. 1*f*).

The effect of desorption pressure (at the discharge outlet of the PSA device P_1^{out} on the concentration and degree of oxygen extraction in the PSA device is shown in Fig. 2. With a decrease of P_1^{out} from $1 \cdot 10^5$ to $0.25 \cdot 10^5$ Pa the fraction of the flow taken for regeneration of the adsorbent decreases (characterized by a backflow coefficient θ), which is ensured by increasing the pressure ratio k_p (if $P^{in} = 2 \cdot 10^5$ and $P_1^{out} = 1 \cdot 10^5$ Pa, $k_p = 2$, and if $P_1^{out} = 0.25 \cdot 10^5$ Pa, $k_p = 8$). As a result, the performance of the device increases (for example, if $t_{ads} = 10$ s, $P^{in} = 2 \cdot 10^5$ Pa, Q increases from 0.25 to 5.2 l/min; and if $P^{in} = 4 \cdot 10^5$ Pa, Q increases from 1.9 to 5.8 l/min). The degree of oxygen extraction η increases from 7 % (Fig. 2*b*, curve *3*) to 61 % if $t_{ads} = 10$ s, $P^{in} = 2 \cdot 10^5$ Pa (Fig. 2*b*, curve *1*), and if $P^{in} = 4 \cdot 10^5$ Pa it increases from 51 % (Fig. 2*d*, curve *3*) to 73 % (Fig. 2*d*, curve *1*). Thus, an increase in η is ensured by a simultaneous increase in P^{in} and decrease in P_1^{out} (i.e. increase in k_p).

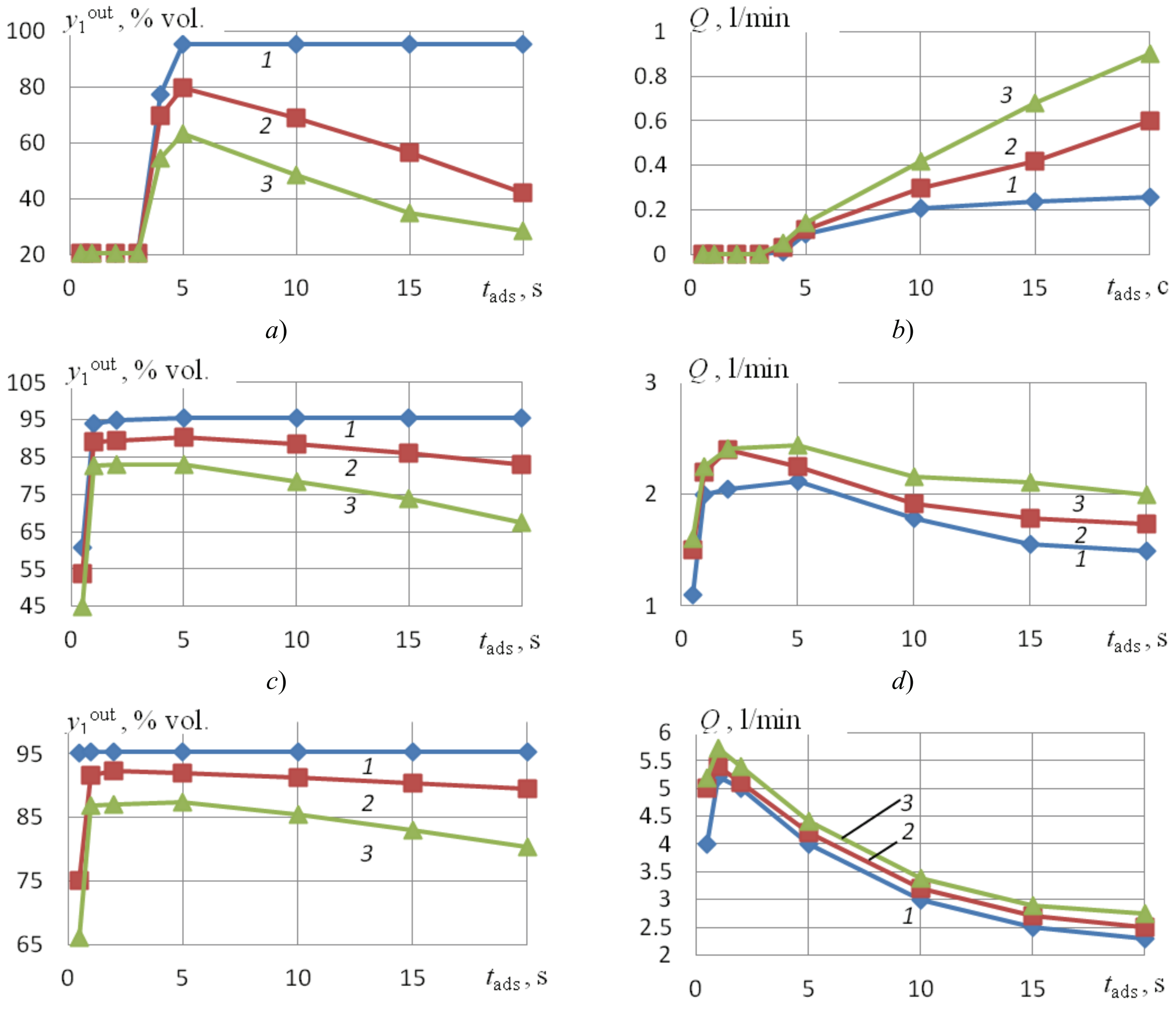
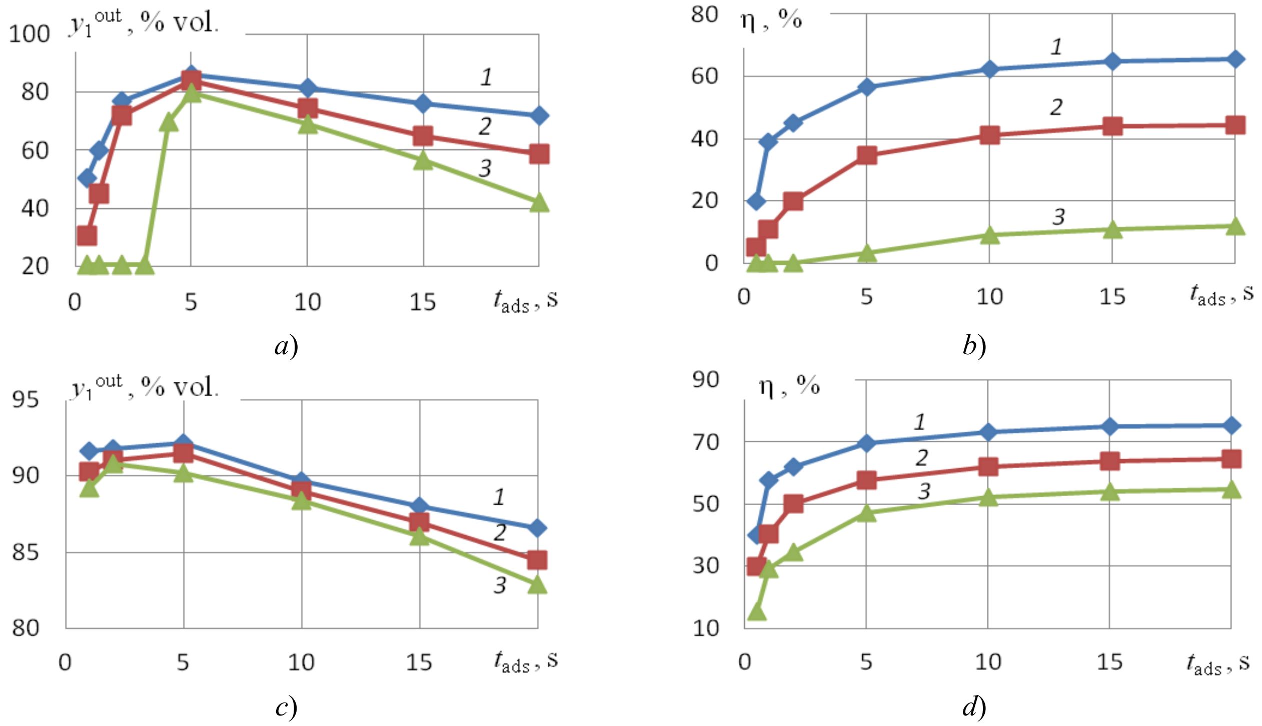


Fig. 1. The dependence of the concentration of production oxygen y_1^{out} (*a*, *c*, *e*) and device performance *Q* (*b*, *d*, *f*) on duration t_{ads} of "adsorption-desorption" half cycle for the compressor inlet pressure $P^{in} = 2 \cdot 10^5$ Pa (*a*, *b*), $4 \cdot 10^5$ Pa (*c*, *d*), $6 \cdot 10^5$ Pa (*e*, *f*) and the temperature of the initial gas-air mixture:

1 – $T_g^{in} = 243$ K; *2* – $T_g^{in} = 293$ K; *3* – $T_g^{in} = 303$ K

It can also be noted that with a decrease in P_1^{out} from $1 \cdot 10^5$ to $0.25 \cdot 10^5$ Pa, oxygen concentration at the device outlet y_1^{out} varies slightly: by ~ 5 % vol. for $P^{in} = 2 \cdot 10^5$ Pa (Fig. 2*a*, curves *1*, *3*) and by ~ 3 % vol. – if $P^{in} = 4 \cdot 10^5$ Pa (Fig. 2*c*, curves *1*, *3*).

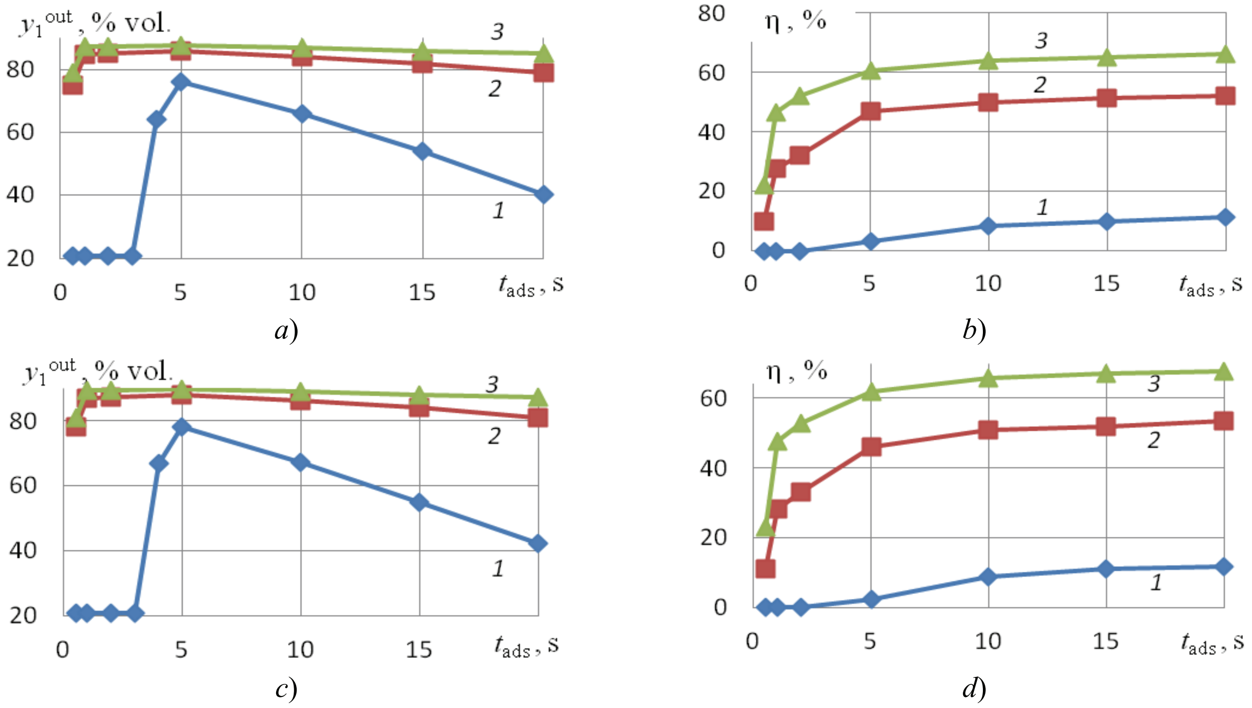
In the study of the influence of the composition of the initial gas-air mixture (oxygen concentration at the device inlet y_1^{in}) on the concentration and degree of oxygen extraction at the PSA device outlet (Fig. 3) the following regularities were found. With an increase in P^{in} from $2 \cdot 10^5$ to $6 \cdot 10^5$ Pa an increase in the gas-air flow rate in the adsorber is observed, respectively, as in the case described in Fig. 1, the time of air enrichment with oxygen is reduced to the maximum achievable concentration. A comparative analysis of the curves in Fig. 3 showed that the change in the concentration of oxygen in the input stream from 19.8 up to 20.3 % vol. causes a change in the maximum oxygen concentration at the PSA outlet: if $P^{in} = 2 \cdot 10^5$ Pa, it varies from 76.2 to 78.6 % vol. (Fig. 3*a*, *c*, curves *1*), as well as the degree of its extraction from 8.2 to 10.1 % (Fig. 3*b*, *d*, curves *1*); if $P^{in} = 4 \cdot 10^5$ Pa, it varies from 83.6 to 85.4 % vol. (Fig. 3*a*, *c*, curves *3*), as well as the degree of its extraction from 62 to 64.2 % (Fig. 3*b*, *d*, curves *3*).



a) *b*)

c) *d*)

Fig. 2. Dependence of concentration y_1^{out} (*a*, *c*) and degree of extraction η (*b*, *d*) of production oxygen on the duration of half cycle t_{ads} if pressure at the compressor outlet $P^{in} = 2\cdot10^5$ Pa (*a*, *b*); $4\cdot10^5$ Pa (*c*, *d*) and pressure at the device outlet: *1* – $P_1^{out} = 0.25\cdot10^5$ Pa; *2* – $P_1^{out} = 0.5\cdot10^5$ Pa; *3* – $P_1^{out} = 1\cdot10^5$ Pa



a) *b*)

c) *d*)

Fig. 3. Dependence of concentration y_1^{out} (*a*, *c*) and degree of extraction of production oxygen η (*b*, *d*) on duration t_{ads} of "adsorption-desorption" half-cycle if oxygen concentration in the initial gas-air mixture y_1^{in} = 19.8 % vol. (*a*, *b*); y_1^{in} = 20.3 % vol. (*c*, *d*) and pressure at the compressor outlet:

1 – $P^{in} = 2\cdot10^5$ Pa; *2* – $P^{in} = 4\cdot10^5$ Pa; *3* – $P^{in} = 6\cdot10^5$ Pa

An increase in P^{in} from $2{\cdot}10^5$ to $6{\cdot}10^5$ Pa provides an increase in maximum oxygen concentration y_1^{out} by ~ 7 % vol. (Fig. 3*a*, *c*, curves *1*, *3*), and the degree of extraction – by more than 6 times (Fig. 3*b*, *d*, curves *1*, *3*).

A study of the effect of changes in time of the degree of valve opening on the performance of a pressure swing adsorption device for air-enriched oxygen

When implementing the step-by-step law of valve opening in order to limit the gas-air flow rate in the frontal layer of the adsorbent, it is necessary to determine the program for changing the degree of their opening in time, ensuring the achievement of maximum values of concentration, degree of extraction, and PSA device performance. The source data for the computational experiments are presented in Table. 2.

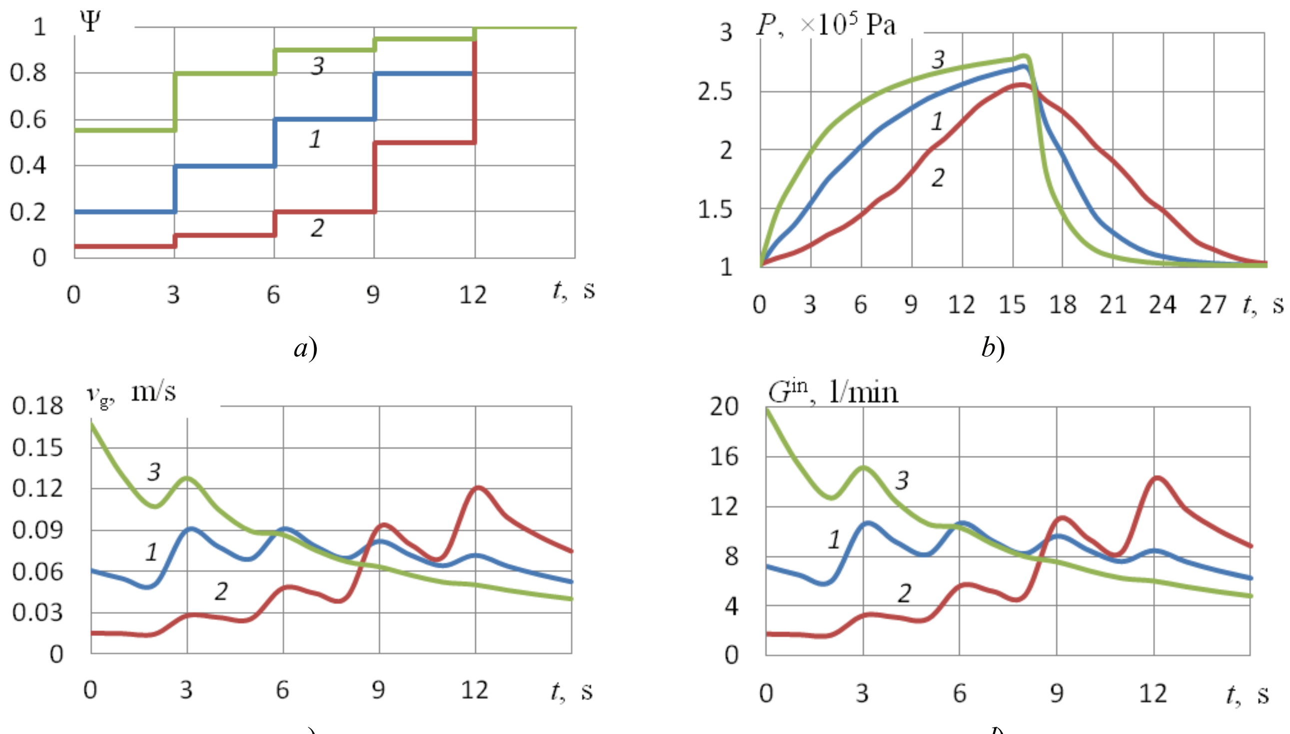
The program of change in time of the degree of opening of the inlet valves can be implemented in accordance with the uniform, convex and concave laws of change. The pressure dynamics in the adsorber, corresponding to the law of the change in time of the degree of valve opening is shown in Fig. 4.

Table 2

The Source data for a computational experiment to study the influence of the law (program) of the degree of opening of the inlet valves in time on the performance of the PSA device

Source data	Nominal values
Gas mixture composition *i*	1 – O_2; 2 – N_2, 3 – Ar
Zeolite adsorbent	NaX
Adsorption limit W_0, sm^3/g	0.17
Parameter *B* for Dubinin equation, ×10^{-6}, 1/K^2	6.55
Design parameters	
The number of adsorbers in the PSA device	2
Adsorber internal diameter D_{A}, m	0.05
Adsorbent layer length H_{L}, m	0.5
Adsorbent granule diameter d_{gr}, mm	2
Reciver volume V_{R}, l	5

Variables	Range of variation	Nominal values
Load		
Capacity of inlet and oulet discharge valves G^{V}, l/min	2–72	18
Controls		
Time t_{c} of adsorption-desorption cycle, s	1–360	30
Pressure at the adsorption stage $P_{\text{ads}}^{\text{in}} \times 10^{-5}$, Pa	2–6	3
Pressure ad the desorption stage $P_{\text{des}}^{\text{in}} \times 10^{-5}$, Pa	0.25–1	1
Backflow coefficient θ, RU	0–2	1.6
Degree of valve opening ψ_{λ}^{j}, RU:		
convex law		0.05; 0.1; 0.2; 0.5; 1.0
uniform law		0.2; 0.4; 0.6; 0.8; 1.0
concave law		0.55; 0.8; 0.9; 0.95; 1.0
Valve full opening time, s		12
Uncertain parameters		
Component concentration in the initial mixture $y_{\text{env},i}$, % vol.	19.8–21.3; 78.2; 0.5–2.0	20.8; 78.2; 1.0
Initial mixture temperature T_{env}, °C	–40 – +40	20



a) *b*) *c*) *d*)

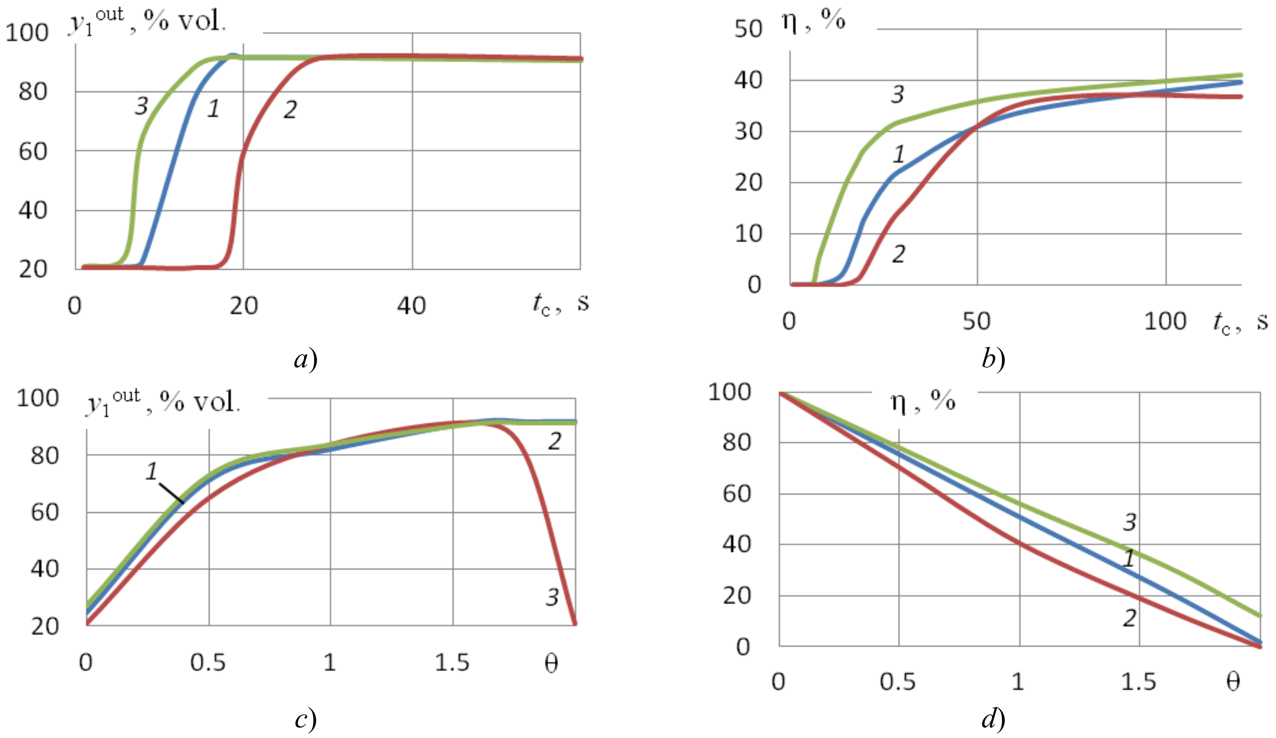
Fig. 4. Dynamics of changes in the degree of opening valves of (*a*), pressure (*b*), velocity (*c*) and inlet flow rate (*d*) in an adsorber in one cycle (0–15 s – adsorption; 16–30 s – desorption) for different laws of change:
1 – uniform; *2* – convex; *3* – concave

When implementing the concave law of valve opening (Fig. 4*b*, curve *3*) an increased rate of pressure build-up in the adsorbent layer is observed, which is explained by a higher opening velocity of the inlet valves (Fig. 4*a*, curve *3*), and, accordingly, higher velocity (Fig. 4*c*, curve *3*) and gas flow rate (Fig. 4*d*, curve *3*) at the outlet to the adsorber if $t = 0 - 6$ s.

An analysis of the dependence of the concentration and degree of production oxygen extraction on the cycle time in the PSA device for various laws of changing the degree of valve opening allows us to conclude that the use of the concave law ensures the achievement of the maximum oxygen concentration $y_1^{\text{out}} = 92$ % vol. at the outlet of the PSA device is much faster than the use of uniform law (14 s against 16 s, Fig. 5*a*, curvese *3*, *1*) and convex law (14 s against 28 s, Fig. 5*a*, curvese *3*, *2*). The degree of extraction using the concave law (Fig. 5*b*, curve *3*) is significantly higher compared to using the uniform law (Fig. 5*b*, curve *1*) and convex law (Fig. 5*b*, curve *2*). In particular, this regularity manifests itself for duration $t_c = 5–30$ s of “adsorption-desorption cycle”. For comparison, for duration $t_c = 20$ s of “adsorption-desorption cycle” we have: *1* – $\eta = 14$ %; *2* – $\eta = 4$ %; *3* – $\eta = 27$ % (Fig. 5*b*).

The influence of the backflow coefficient θ on the concentration and degree of extraction of production oxygen for different laws of change in time of the degree of opening of the valves is less significant than, for example, the effect of the duration of the “adsorption-desorption” cycle (Fig. 5*c*, *d*). If $\theta = 0.5$, the difference between the values of the degrees of extraction when using concave and convex laws is 11 %, and for $\theta = 1.5$ this difference increases to ~ 18 % (Fig. 5*d*, curves *3*, *2*).

The analysis of dependence y_1^{out} and η on temperature T_{g}^{in} and impurity concentration y_3^{in} in the initial gas-air mixture indicates that the oxygen concentration at the outlet of the PSA device is practically independent of the type of law of the change in time of the degree of opening of the inlet valves (Fig. 6*a*, *c*), and the difference between the values of the degrees of extraction (Fig. 6*b*, *d*) is proportional to the performance of the installation under various laws and is practically independent of T_{g}^{in} and y_3^{in}.

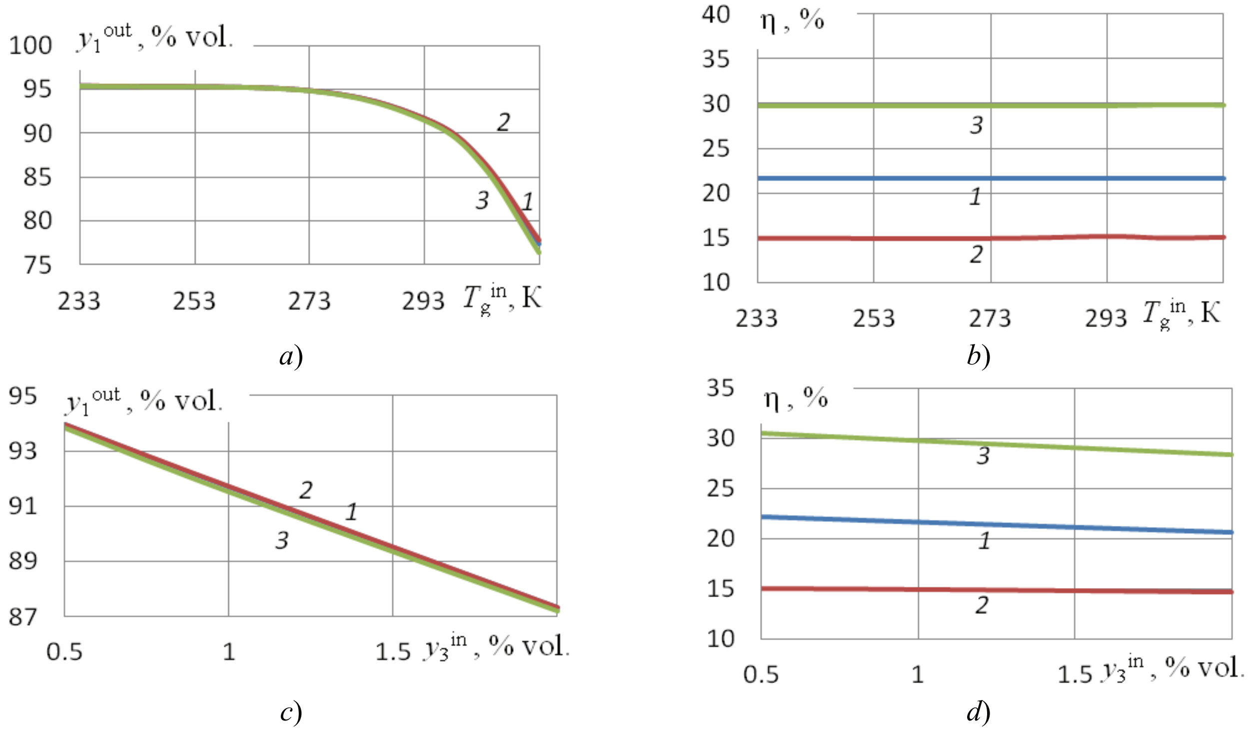


a) *b*)

c) *d*)

Fig. 5. Dependence of concentration y_1^{out} (*a*, *c*) and degree of extraction of production oxygen η (*b*, *d*) on duration t_c (*a*, *b*) of "adsorption-desorption" cycle and backflow coefficient θ (*c*, *d*) for different laws of change in time of the opening degree of valves:

1 – uniform; *2* – convex; *3* – concave

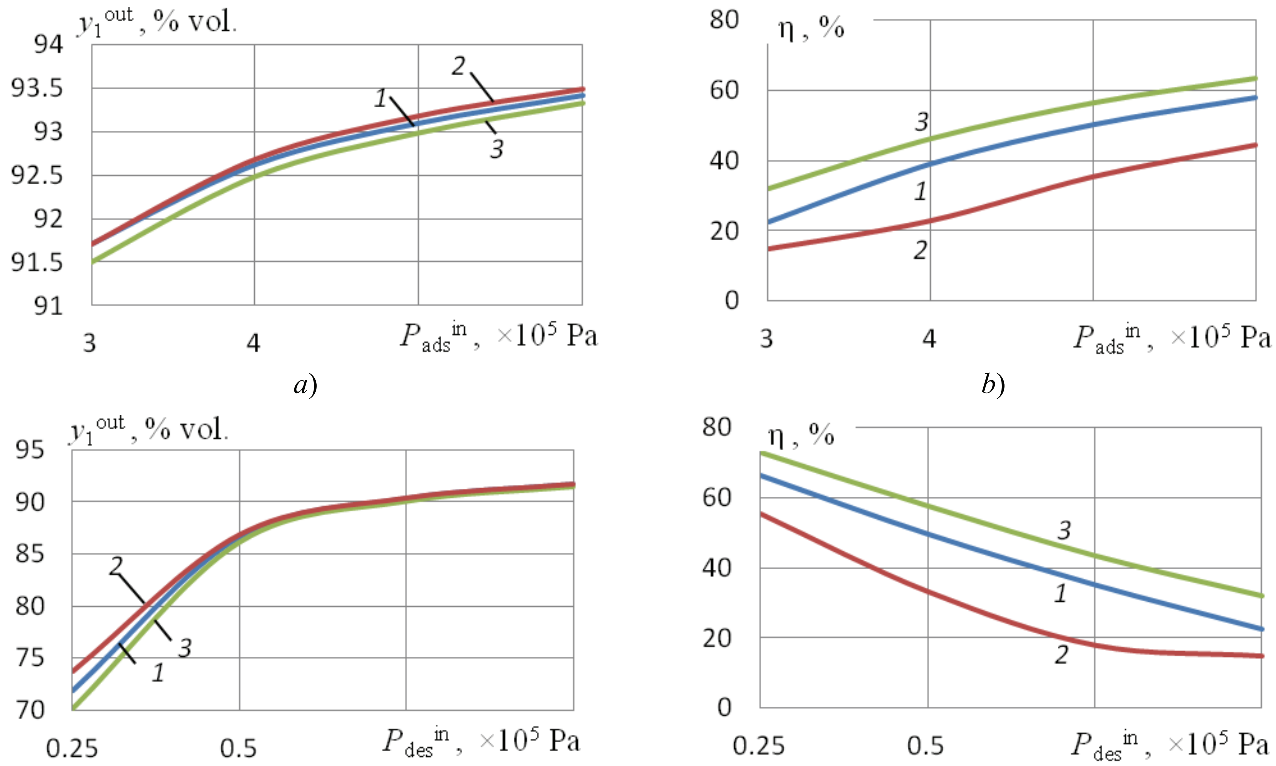


a) *b*)

c) *d*)

Fig. 6. Dependence of concentration y_1^{out} (*a*, *c*) and degree of extraction η (*b*, *d*) of production oxygen on temperature T_g^{in} (*a*, *b*) initial air-gas mixture and concentration y_3^{in} (*c*, *d*) of impurities in the initial gas-air mixture with various laws of change in time of the degree of opening of the valves:

1 – uniform; *2* – convex; *3* – concave



a) *b*)

c) *d*)

Fig. 7. Dependence of concentration y_1^{out} (*a*, *c*) and degree of extraction η (*b*, *d*) of production oxygen on pressures P_{ads}^{in} (*a*, *b*), P_{des}^{in} (*c*, *d*) at the stages of adsorption and desorption, respectively, with different laws of change in time of the degree of opening of the valves:
1 – uniform; *2* – convex; *3* – concave

From the analysis of the dependencies y_1^{out} and η on pressure at the adsorption stag P_{ads}^{in} it follows that the oxygen concentration at the outlet of the PSA device during the transition from concave to convex law changes less than 1% vol. (Fig. 7*a*). With an increase in P_{ads}^{in} there is also an increase in η (Fig. 7*b*) y_1^{out}, as the equilibrium nitrogen concentration in the adsorbent increases (Fig. 7*a*) and, so does the efficiency of gas separation [1–3]. The latter is largely due to the increased productivity of the PSA device (an increase in P_{ads}^{in} contributes to a decrease in the return flow coefficient θ and, respectively, to an increase in the production flow extraction).

The analysis of dependencies y_1^{out} and η on pressure values at the desorption stage P_{des}^{in} shows that the dependence of the oxygen concentration at the outlet of the PSA device on the type of valve opening law appears only if P_{des}^{in} is less than 0.5×10^5 Pa (Fig. 7*c*). The difference between the values of the degrees of extraction (рис. 7*d*) is proportional to the performance of the device under different laws of change in time of the degree of opening of the valves. The similar character of the influence on y_1^{out} and η have changes in P_{ads}^{in} and P_{des}^{in}, which is explained by a change in the coefficient of pressure ratio k_p in almost the same range: or example, with an increase in pressure at the adsorption stage k_p changes from 3 to 6, and with a decrease in pressure at the desorption stage, it changes from 1 to 4.

Conclusions

The studies of heat and mass transfer processes in pressure swing adsorption processes for oxygen-enriched air established a rational law of time variation in the degree of opening of the inlet and outlet valves of PSA devices (as well as its effect on the performance of PSA devices), which, along with resource-saving expensive adsorbent, provides the highest degree of extraction of oxygen from atmospheric air. The results can be used to optimize and optimize the design of cyclic adsorption processes and resource-saving PSA devices for the separation and purification of gas mixtures

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