MSC 65P99 **DOI: 10.14529/mmp200201**

THE OPTIMAL DESIGN OF PRESSURE SWING ADSORPTION PROCESS OF AIR OXYGEN ENRICHMENT UNDER UNCERTAINTY

E.I. Akulinin*[1]*, O.O. Golubyatnikov*[1]*, D.S. Dvoretsky*[1]*, S.I. Dvoretsky*[1]*,
[1]Tambov State Technical University, Russian Federation
E-mails: akulinin-2006@yandex.ru, golubyatnikov_ol@mail.ru, dvoretsky@tambov.ru, sdvoretsky@mail.tstu.ru

The paper formulates and studies the problem of optimal (by the criterion of profits from oxygen production) design of a pressure swing adsorption (PSA) unit for air oxygen enrichment under partial uncertainty of the source data (the air composition, temperature, atmospheric pressure) with limitations on oxygen purity, unit capacity, and resource saving granular adsorbent. A heuristic iterative algorithm was developed for solving an optimal design problem under partial uncertainty of the source data. An auxiliary optimization problem related to the class of nonlinear programming problems (assuming the approximation of continuous control functions at the stages of the adsorption-desorption cycle by step-functions) was formulated and then solved by the sequential quadratic programming method. The problem of optimal design was solved for the range of PSA units with a capacity of 1 to 4 l/min allowing to obtain oxygen with a purity of 40 to 90% vol. According to the findings, we analyze the most promising operational and design parameters ensuring the maximum profit in the operation of the PSA unit, taking into account the saving of the granular adsorbent. It was established that the introduction of limitations on the gas flow rate in the frontal layer of the PSA unit adsorbent allows to increase the reliability of its operation and the adsorbent service life.

Keywords: pressure swing adsorption; zeolite; mathematical modelling; optimization; design; uncertainty.

Introduction

When calculating and designing technological processes, the so-called indefinite ("inaccurate") information is often used. Such an information involves physico-chemical parameters, characteristics of the source/"raw" substances, structural/geometrical indicators of technological equipment fragments, external operating conditions of the process, financial/cost data, etc. The information indirectly has a significant impact on the quality of the technological process characterized by known technical and economic indicators, e.g. profit [1, 2]. A quantitative account of a number of specified "inaccurate"/random factors plays a crucial role in the design of technological processes and units under partial (incomplete) uncertainty.

In the design accounting for uncertain source data is necessary to formulate the problem of the optimal design on technological processes and units, which will allow to create reliable industrial designs functioning effectively regardless of random variation of uncertain parameters within specified limits.

In recent decades, cyclic adsorption processes and, in particular, pressure swing adsorption (PSA) processes have become the most common way of separating gas mixtures and concentrating the target products in them. The PSA processes are widely used in industry for the non-heating separation of hydrocarbons, extraction of methane, carbon dioxide, hydrogen from hydrogen-containing process streams, oxygen and nitrogen from atmospheric air [3–5]. The advantages of PSA units are their autonomy, mobility, reliability, quick access to the stationary periodic mode, and the possibility of full automation.

In the field of adsorption separation of multicomponent gas mixtures, one of the urgent tasks is air oxygen enrichment, since the annual growth in oxygen demand is on average ∼4–5% due to the increased demand in ferrous metallurgy, chemical industry, aluminum production, and medicine. At the same time, a significant proportion of consumers use not so much pure oxygen in their activity, compared to the air enriched with oxygen from 40 to 90% vol. [6–8].

When calculating and designing PSA units for air separation and oxygen concentration, uncertain parameters are air composition, temperature and atmospheric pressure. Parameters of the mathematical model are diffusion coefficients, heat and mass transfer, thermal conductivity, etc. The parameters can vary randomly in certain ranges depending on the unit operating conditions and, in particular, on the climatic and geographical characteristics. Therefore, during the operation of PSA medical concentrators in closed rooms, the ambient temperature can vary from 293 to 303 K, the pressure can vary: from $0{,}75\times10^5$ to $1{,}0\times10^5$ Pa at an altitude of 2 km above sea level, the oxygen concentration in the air can vary: from 18 to 21%, while during the operation of onboard oxygen units the ranges of changes in similar parameters be much larger [9].

The goal of this work is to pose the problem on the optimal design of a two-sorber PSA unit for air oxygen enrichment under partial uncertainty of the source data, develop a heuristic iterative algorithm for determining the design parameters and operating variables of the PSA unit when maximum oxygen production is achieved and the process requirements for oxygen purity are met, as well as the unit capacity and resource-saving from the adsorbent granules abrasion.

1. The Analysis of Pressure Swing Adsorption Process of Air Oxygen Enrichment as a Design Object

Suppose that the atmospheric air containing oxygen O_2 in the amount of 18–21% vol., nitrogen 78 – 80% vol., argon and other impurities 1 – 2% vol. in the arount of the technological process of separating the atmospheric air is carried out in a two-adsorber PSA unit with the granulated synthetic zeolite adsorbent 13X [10]. The atmospheric air is supplied to the unit after preliminary drying with an overpressure in the range from 2×10^5 to 6×10^5 Pa. In order to prevent the abrasion of the adsorbent granules, the adsorbers pressure is increased by “careful” opening the control inlet valves [9]. From the first adsorber the main part of the production stream of oxygen-enriched air is sent to the consumer, and the other part of the stream is sent counter-current to the second adsorber for washing the adsorbent layer and desorbing mainly nitrogen. At the same time, in the second adsorber, the pressure is reduced to atmospheric by opening the exhaust control valve, through which the desorbed stream is discharged for further processing. In the technological scheme, the adsorbers work alternately.

When predominantly adsorbing N_2 and O_2 with the granular adsorbent 13X, the following mass and heat exchange processes take place in the adsorbers of the PSA unit:

1) N_2, O_2, Ar diffusion in the gas-air mixture flow; 2) N_2, O_2, Ar mass transfer and heat exchange between the gas phase and the adsorbent; 3) N_2, O_2, Ar adsorption on the surface and in the micropores of the zeolite adsorbent granules with the heat release; 4) N_2, O_2, Ar desorption from the micropores and from the surface of granules with the heat absorption during the adsorbent regeneration.

When developing a mathematical model of the dynamics of air oxygen enrichment, we assume the following: 1) the initial gas-air mixture is 3-component (contains 1 – oxygen O_2 with a concentration of 18 – 21% vol., 2 – nitrogen N_2 with a concentration of 78 – 80% vol., 3 – argon Ar and impurities with a concentration of 1 – 2% vol.) and considered as an ideal gas, which is quite acceptable at pressures in the adsorber up to 200×10^5 Pa [11]; 2) the adsorptive diffusion (oxygen, nitrogen, argon) and the heat propagation in the gas and solid phases occur only in the axial direction of the gas mixture flow in the adsorber (along the length of the adsorbent layer) [6–8]; 3) the granulated zeolite 13X with a diameter of 1 mm is used as an adsorbent [4]; 4) the adsorption equilibrium (adsorption isotherm) is described by the Dubinin–Radushkevich equation [12]; 5) the desorption branches of adsorption isotherms (N_2, O_2, Ar) on zeolite 13X coincide with the adsorption branches [4].

The mathematical model of the dynamics of the cyclic adsorption process for separating atmospheric air and oxygen concentration is a system of nonlinear partial differential equations of parabolic type with corresponding initial and boundary conditions for the stages of the adsorption-desorption cycle and formulas for calculating the model parameters [13].

In order to solve the equations of the mathematical model of dynamics, we use the method of lines [14] in the Matlab software environment. Solving the equations of the model [13] was carried out before the onset of the cyclic steady state (CSS) mode [6–8, 15] in the PSA unit operation, i.e. under the condition $|y_{1,n}^{out} - y_{1,n-1}^{out}| \leq 10^{-3}$, which is reached approximately after n ≈20 – 30 of adsorption-desorption cycles [13, 15].

The analysis of the mathematical model adequacy was carried out with experimental and calculated data using the actual root-mean-square error, which was 5,2%, allowing to use the mathematical model for technological calculation, optimization of cyclic adsorption processes and designing PSA units for air separation and oxygen concentration.

Previously conducted numerical studies of the dynamics of cyclic adsorption processes of air oxygen enrichment made it possible to establish that high gas flow rates are achieved in the adsorbent frontal layer above 0,15–0,25 m/s and aerodynamic impacts occur when the inlet and outlet valves are fully open, which leads to mechanical abrasion and dusting of the granulated adsorbent [10, 16]. This fact must be taken into account when solving problems on the optimal design of PSA units in the separation of gas mixtures. The speed limit in the adsorbent frontal layer can be achieved by controlling the opening degree of the inlet and outlet valves of the PSA unit according to a certain law, which is found as a result of solving the optimization problem. In addition, we esteblish the most dangerous perturbations ξ: the composition y_{env}, temperature T_{env} and pressure P_{env} of atmospheric air [17]; the most effective mode parameters u: pressure P^{in} at the compressor outlet, duration of the adsorption stage or half-cycle duration $t_{ads} = t_c/2$, backflow ratio θ, time variable programs for the degree of opening the inlet ψ_1^λ and outlet ψ_2^λ, valves $\lambda = \overline{1,m}$, design parameters d of the PSA unit: the adsorber internal diameter D_A, the height of the adsorbent layer L, the adsorbent granule diameter d_{gr}, the capacity of the inlet and outlet valves K_v; the output variables z_{st} of the PSA unit in the CSS mode: concentrations of oxygen $y^{out}_{1,st}$, nitrogen $y^{out}_{2,st}$ and argon $y^{out}_{3,st}$ in the product flow, the unit capacity G^{out}_{st}, the extracting degree η_{st} of oxygen and profit $\varphi(d, u, z_{st}, \xi)$ from the unit operation during the life cycle LT = 10 years.

Time variable programs for the degree of opening the inlet and waste valves $\psi^{\lambda}_1(t_\lambda)$, $t_\lambda \in [0, t_{ads}]$ and outlet valves $\psi^{\lambda}_2(t_\lambda)$, $t_\lambda \in [t_{ads}, t_c]$ in the time interval $[0, t_c]$ will be approximated by piecewise constant (step) functions: $\psi^{\lambda}_1 = \psi_1(\tau_\lambda)$, $\tau_\lambda \in [0, t_{ads}]$, $\lambda = \overline{1, m}$; $\psi^{\lambda}_2 = \psi_2(\tau_\lambda)$, $\tau_\lambda \in [t_{ads}, t_c]$, $\lambda = \overline{1, m}$;

The purpose of the PSA unit for air separation is the production of oxygen with a maximum φ profit, with an oxygen concentration not lower than a predetermined $y^{out}_{1,def}$ % vol. and in a given amount (the PSA unit capacity is the flow rate G^{out} of the production air flow with a given oxygen concentration y^{out}_1 must not be lower than the specified one G^{out}). As a criterion for the optimal design of the PSA unit under partial uncertainty, the average profit value φ from oxygen production was used, i.e. $M_\xi(\varphi(d, u, z_{st}, \xi))$, where M_ξ is the mathematical expectation symbol.

The profit φ, million \$/year, which can be obtained from oxygen production during the life cycle LT = 10 years of the PSA unit, was calculated according to the formula proposed in [15]:

$$\varphi(d, u, z_{st}, \xi) = P_{val} LT - OC \cdot LT - C;\ \text{product value } P_{val},\ \$/\text{year:}$$
$$P_{val}(d, u, z_{st}, \xi) = Q_{prod}(d, u, z_{st}, \xi) \cdot p;\ \text{operation costs } OC,\ \$/\text{year:}$$
$$OC(d, u, \xi) = Q_{in}(d, u, \xi) \cdot W_c(u, \xi) \cdot EC;$$
$$W_c(u, \xi) = (\frac{\gamma}{\gamma - 1}) P_0 \frac{T_{env}}{T_0} [(\frac{P^{in}}{P_{env}})^{\frac{\gamma-1}{\gamma}} - 1];\ \text{capital expenditures } C,\ \$:$$
$$C(d) = V_A(d) C_{ads} + C_{col} + C_{st} + C_{com} + C_{deh} + C_{PLC} + C_{val} + C_{ret} + C_{th} + C_{other},$$

where Q_{in} is the average cost of entry into the unit, m^3/year; Q_{prod} is the unit capacity, m^3 product/year; V_A is the adsorbent volume, m^3; W_c is the adiabatic compressor power, J/m^3; γ is the adiabatic index for the gas mixture; T_0, P_0 is air temperature and pressure under normal conditions; p is the product cost, \$/m^3; EC is energy costs, \$/J; C_{col} is the adsorber cost, \$; C_{ads} is the adsorbent cost, \$/m^3; C_{st} is the receiver cost, \$; C_{deh} is the dehydrator cost, \$; C_{com} is the compressor cost, \$; C_{th} is the throttle cost, \$; C_{PLC} is the cost of programmable logic controller, \$; C_{val} is the cost of controlled valves, \$; C_{ret} is the cost of return valves, \$; C_{other} is the cost of other equipment, \$.

2. Statement of the Problem on Optimal Design of Pressure Swing Adsorption Process of Air Oxygen Enrichment under Uncertainty

Suppose that the vector $\xi = \{y_{env}, T_{env}, P_{env}\}$ with indefinite parameters belongs to a certain domain $\Xi = \{\xi^- \le \xi \le \xi^+\}$, $\xi \in \Xi \subset E^{n_\xi}$, where n_ξ is the dimension of the vector ξ with indefinite parameters, $n_\xi = 3$. The problem on the optimal design of the PSA unit according to the criterion $M_\xi(\varphi(d, u, z_{st}, \xi))$ is formulated as follows: it is required to determine the design $d^* = \{D^*_A, L^*, K^*_v\}$ and regime parameters $u^* = \{t^*_{ads}, P^{in*}, \psi^{\lambda*}_1, \psi^{\lambda*}_2, \lambda = \overline{1, 20}\}$ such that the profit $\varphi(d, u, z_{st}, \xi)$ from operating the PSA unit in the CSS mode for LT = 10 years reaches the maximum value, i.e.

$$I(d^*, u^*) = \max_{d,u} M_\xi(\varphi(d, u, z_{st}, \xi)) \qquad (1)$$

with connections in the form of mathematical model equations of the cyclic adsorption process of air oxygen enrichment [13] and restrictions on:

– the purity $y_{1,st}^{out}$ of product oxygen

$$\max_{\xi\in\Xi}\{g_1(d,u,\xi)=y_{1,def}^{out}-y_{1,st}^{out}(d,u,\xi)\}\le 0; \tag{2}$$

– the capacity G_{st}^{out} of the PSA unit

$$\max_{\xi\in\Xi}\{g_2(d,u,\xi)=G_{def}^{out}-G_{st}^{out}(d,u,\xi)\}\le 0; \tag{3}$$

– the flow rate of the gas mixture ν_g in the adsorbent frontal layer

$$\max_{\xi\in\Xi}\{g_3(d,u,\xi)=\max_{\tau\in[0,t_c]}\nu_g(d,u,\xi,\tau)-\nu_g^+\}\le 0; \tag{4}$$

– the pressure drop in the adsorbent layer at the adsorption and desorption steps

$$\max_{\xi\in\Xi}\{g_4(d,u,\xi)=P_{env}-P_{ads}^{out}(d,u,\xi)\}\le 0; \tag{5}$$

$$\max_{\xi\in\Xi}\{g_5(d,u,\xi)=P_{env}-P_{des}^{out}(d,u,\xi)\}\le 0; \tag{6}$$

– regime ranges u

$$1\le t_{ads}\le 120s, 2\times 10^5\le P^{in}\le 6\times 10^5Pa, 0\le \psi_j^\lambda\le 1, j=1,2; \lambda=\overline{1,20}; \tag{7}$$

– ranges in design parameters d

$$0,02\le D_A\le 0,15m, 0,15\le L\le 0,8m, 5\le K_v\le 20l/min; \tag{8}$$

– ranges of uncertain parameters $\xi\in\Xi$

$$\begin{gathered}18\le y_{env,1}\le 21\%vol., 78\le y_{env,2}\le 80\%vol., 1\le y_{env,3}\le 2\%vol.,\\ 293\le T_{env}\le 303K, 0,75\times 10^5\le P_{env}\le 1\times 10^5Pa,\end{gathered} \tag{9}$$

where ν_g^+ is the maximum allowable flow rate of the gas mixture in the adsorbent frontal layer.

The functions $g_1(\cdot)$, $g_2(\cdot)$ in restrictions (2), (3) were calculated by solving the mathematical model equations for the dynamics of the cyclic adsorption process of air oxygen enrichment to the CSS mode of the PSA unit, and the functions $g_3(\cdot)$, $g_4(\cdot)$, $g_5(\cdot)$ in restrictions (4) – (6) were calculeted on the time interval $[0,t_c]$. The physical meaning of limiting the maximum value of air velocity ν_g in the adsorbent frontal layer is to protect the granular adsorbent from destruction due to aerodynamic impact with full abrupt opening of the control valves of the PSA unit, which increases the service life of the adsorbent.

Since the probability of the indefinite parameters to accept certain values from the specified ranges $\xi^-\le\xi\le\xi^+$ is unknown, it is assumed that they are uniformly distributed.

The formulated optimization problem (1) – (9) under partial uncertainty of parameters $\xi\in\Xi\subset E^3$ belongs to the class of non-linear programming problems, which will be solved using the developed heuristic iterative algorithm and the method of sequential quadratic programming in the Matlab software environment (solver fmincon) [18].

3. An Algorithm for Solving the Problem on Optimal Design of Pressure Swing Adsorption Process of Air Oxygen Enrichment under Uncertainty

A priori, we introduce the set $S_1=\{\xi^i:\xi^i\in\Xi, i\in J_1\}$ of approximation points and the set S_2 of "critical" points at which restrictions (2) – (6) of problem (1) – (9) can be violated. Suppose that the functions $g_j(\cdot)$, $j = \overline{1,5}$ are convex. It is advisable to include the corner points ξ_k^-, ξ_k^+, $k = 1, 2, 3$ of the uncertainty region $\Xi \subset E^3$ in the initial set of critical points $S_2^{(0)}$.

The auxiliary problem (A) is formulated as follows: it is required to determine the maximum value $\hat{I}(d, u)$ of the objective function $I(d, u)$, design $\hat{d} \in D$ and regime $\hat{u} \in U$ parameters such that

$$\hat{I}(d, u) = \max_{d,u} \sum\nolimits_{i \in J_1} \omega_i \varphi(d, u, z_{st}, \xi^i) \tag{A}$$

with the connections in the form of the mathematical model equations of the cyclic adsorption process of air oxygen enrichment [13] and the restrictions $g_j(\cdot)$, $j = \overline{1,5}$ calculated at the approximation points $g_j(d, u, z_{st}, \xi^i)$, $j = \overline{1,5}$, $\xi^i \in S_1$, $i \in J_1$, at the critical points $g_j(d, u, z_{st}, \xi^l)$, $j = \overline{1,5}$, $\xi^l \in S_2$, $i \in J_2$, where ω_i is the weight coefficients satisfying the conditions of $\omega_i \geq 0$, $\sum_{i \in J_1} \omega_i = 1$. Since the probability that the uncertain parameters take some values from the given ranges $\xi^- \leq \xi \leq \xi^+$is unknown, it is assumed that the parametrs are distributed in accordance with the equiprobable law. Then the coefficients ω_i are the same for all approximation points ξ^i, $i \in J_1$, i.e. $\omega_i = 1/K_{J_1}$, $i = \overline{1, K_{J_1}}$, $i \in J_1$.

The auxiliary optimization problem (A) belongs to the class of nonlinear programming problems, which was solved by the method of sequential quadratic programming.

The Algorithm. Step 1. The initial number $\nu = 1$, the initial sets of approximation points ξ^i, $i \in J_1$, $\xi^i \in S_1$ and critical points $S_2^{(\nu-1)} = \{\xi^l : \xi^l \in \Xi, l \in J_2^{(\nu-1)}\}$, as well as the initial approximations of the design parameters $d^{(0)}$ and regime parameters $u^{(0)}$. The initial set of critical points $S_2^{(0)}$ is formed by the corner points ξ_k^-, ξ_k^+, $k = 1, 2, 3$, and the uncertainty regions Ξ under the assumption of convexity of functions $g_j(d, u, \xi)$, $j = \overline{1,5}$, describing restrictions (2) – (6).

Step 2. Using the method of sequential quadratic programming, find the solution to the auxiliary problem (A) and determine the values $I(d^{(\nu)}, u^{(\nu)})$ and vectors $d^{(\nu)}$, $u^{(\nu)}$.

Step 3. In order to determine new critical points where restrictions (2) – (6) $g_j(d^{(\nu)}, u^{(\nu)}, z_{st}, \xi)$, $j = \overline{1,5}$, $\xi \in \Xi$ are violated, solve five extreme problems of the form $\max\limits_{\xi} g_j(d^{(\nu)}, u^{(\nu)}, z_{st}, \xi)$, $\xi^- \leq \xi \leq \xi^+$, $j = \overline{1,5}$ and find five points $\xi_1^{(\nu)}$, $\xi_2^{(\nu)}$,...,$\xi_5^{(\nu)}$, which deliver the maximum to the functions $g_j(d^{(\nu)}, u^{(\nu)}, z_{st}, \xi)$, $j = \overline{1,5}$, respectively.

Step 4. Form a new set of critical points: $S_2^{(\nu)} = S_2^{(\nu-1)} \bigcup R^{(\nu)}$, $R^{(\nu)} = \{\xi_1^{(\nu)}, \xi_2^{(\nu)}, ..., \xi_5^{(\nu)} : g_j(d^{(\nu)}, u^{(\nu)}, z_{st}, \xi_1^{(\nu)}, \xi_2^{(\nu)}, ..., \xi_5^{(\nu)} > 0, j = \overline{1,5}\}$. If the set $R^{(\nu)}$ is empty, then the solution to the problem $d^* = d^{(\nu)}$, $u^* = u^{(\nu)}$ is obtained at the ν-th iteration and the algorithm finishes its work; otherwise, we set $\nu = \nu + 1$ and go to Step 2.

4. The Findings on the Problem of Optimal Design on Pressure Swing Adsorption Process of Air Oxygen Enrichment under Uncertainty

Optimal design problem (1) – (9) was solved for the series of PSA units with a capacity of 1 to 4 nl/min, which allow to produce oxygen with a purity of 40 to 90% vol.

Table gives the source data for problem (1) – (9), based on the analysis of the average cost of PSA component units according to the Yandex.market portal.

Table

The source data for solving problem (1) – (9)

Oxygen concentration $y^{out}_{1,def} = 40, 65, 90\%$ vol.	Product cost, $p = 700$ \$/m^3
Capacity of the unit $G^{out}_{def} = 1, 2, 4$ Nl/min	Cost of return valves, $C_{ret} = 5$ \$
Velocity at the frontal layer of the adsorbent $\nu^+_g = 0,2$ m/s	Cost of adsorber, $C_{col} = 15$ \$
Return flow ratio $\theta = 1,8$	Cost of controlled valves, $C_{val} = 75$ \$
Diameter of the adsorbent granules $d_{gr} = 1$ mm	Cost of adsorbent, $C_{ads} = 5$ \$/ kg or 3650 \$/m^3
Life cycle of the unit, $LT = 10$ years	Cost of receiver, $C_{st} = 7,5$ \$
Energy costs, $EC = 1,12 \times 10^{-6}$ \$/J	Cost of dehydrator, $C_{deh} = 15$ \$
Cost of programmable logic controller, $C_{PLC} =$ 500 \$	Cost of compressor, $C_{com} = 470$ \$
Cost of other equipment, $C_{other} = 50$ \$	Cost of throttle, $C_{th} = 7,5$ \$

The findings on the optimal design problem (Fig. 1) allow to conclude that, with the same required capacity of the PSA unit G^{out}_{def}, an increase in the required oxygen concentration $y^{out}_{1,def}$ leads to a slight (less than 5%) decrease in the profit (Fig. 1a). With an increase in the PSA unit capacity, profits grow linearly (Fig. 1b). Therefore, obtaining high-purity oxygen with the same capacity is more profitable than obtaining low-purity oxygen. Let us compare two different oxygen concentrators for medical purposes: 1) with a given capacity $G^{out}_{def} = 2$ Nl/min and concentration $y^{out}_{1,def} = 90$ % vol.; 2) with a given capacity $G^{out}_{def} = 2$ Nl/min, and $y^{out}_{1,def} = 40$ % vol. A feature of medical oxygen concentrators is the ability to dilute the gas stream leaving the PSA unit with a high oxygen concentration to the required concentration by mixing with pre-filtered atmospheric air. When diluting the output stream in option 1), a mixture with a concentration of 40% vol. and flow rate of 7,26 Nl/min will be obtained, while in option 2) a mixture with a concentration of 40% vol. and flow rate of 2 Nl/min will be received. Therefore, the capacity of the PSA unit (with the implementation of option 2) will increase by 3,6 times with insignificantly increasing costs by 1 – 2% (due to the need to supply additional filtered air at atmospheric pressure).

The analysis of the graphs in Fig. 2 indicates that the optimal programs for opening the unit valves (Fig. 2a) obtained by solving problem (1) – (9) make it possible to provide a "safe" flow rate in the frontal layer of the adsorbent $\nu_g < \nu^+_g = 0,2$ m/s [16] (Fig. 2b). It is seen that with an increase in the set unit capacity G^{out}_{def}, a "careful" opening of the valves (an increase in the number of stages) is required to fulfill the restriction (2) (Fig. 2a).

Conclusions

The problem of optimal design of the PSA unit for air oxygen enrichment was formulated and solved under the interval uncertainty in the composition of atmospheric air, temperature and ambient pressure. A heuristic iterative algorithm was developed to solve the optimization problem taking into account the optimality of profits from oxygen production and the requirements of the technological regulations for oxygen purity, PSA unit capacity and resource saving of the adsorbent from the abrasion of the granules.

The formulation of the optimization problem under the conditions of partial uncertainty of the source data and the developed algorithm for its solution can be used

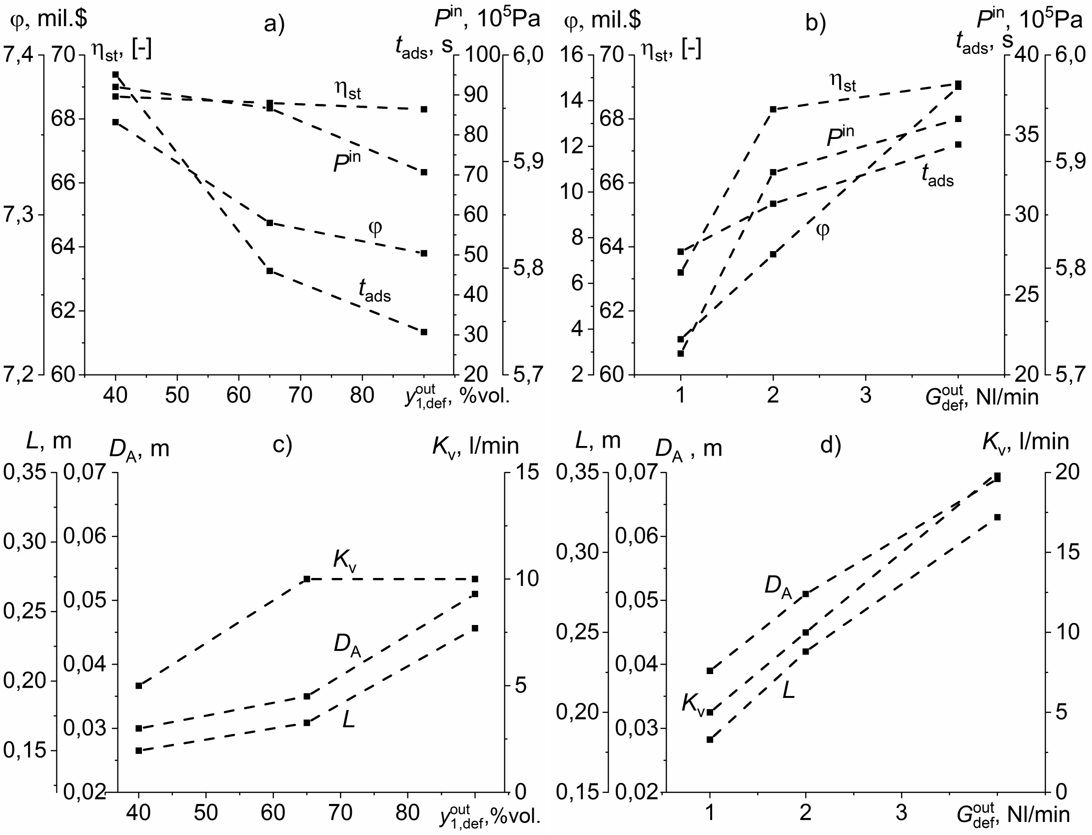

Fig. 1. Optimal values of regime (a, b) and design (c, d) parameters for different values of restrictions a), c) shows per production oxygen concentration $y^{out}_{1,def}$ and $G^{out}_{def} = 2$ Nl/min; b), d) shows per the unit capacity G^{out}_{def} and $y^{out}_{1,def} = 90$ % vol

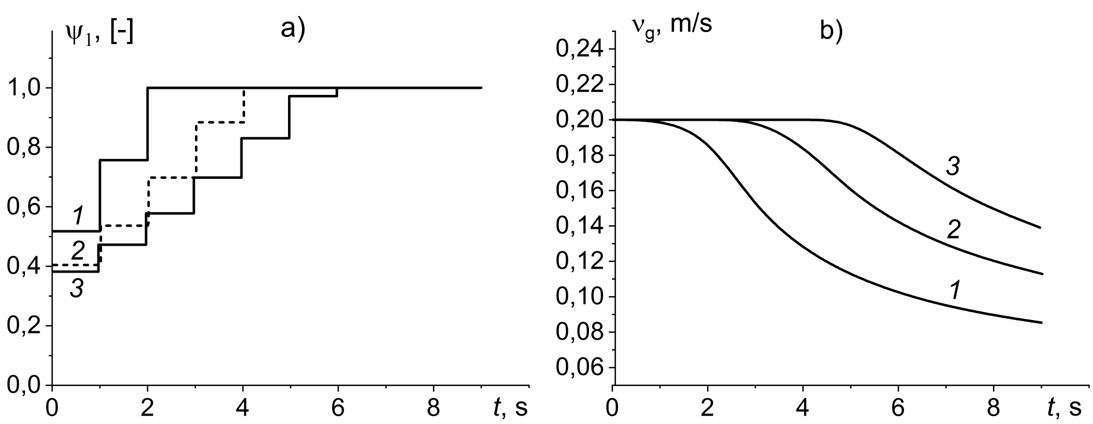

Fig. 2. Dynamics of the opening degree on the unit inlet valves (a) and the flow rate in the frontal layer of the adsorbent (b) with the optimal values of the design and operating parameters: $y^{out}_{1,def} = 90$ % vol., $G^{out}_{def} = 1(1), 2(2), 4(3)$ Nl/min

to upgrade existing units and design new resource-saving PSA units for the separation and purification of multicomponent gas mixtures in which it is necessary to use expensive or unique adsorbents, as well as to ensure the normal operation of the unit in the entire interval of random changes in the values of uncertain parameters.

Acknowledgements. *The work was supported by the Ministry of Science and Higher Education of Russia under the Russia President grant MK-1604.2020.8.*

References

1. Chistyakova T.B., Razygrayev A.S., Polosin A.N., Araztaganova A.M. Joint Innovative IT Projects in the Field of Production of Polymeric Sheet Materials. *Proceedings of the 2016 IEEE V Forum "Strategic Partnership of Universities and Enterprises of Hi-Tech Branches (Science. Education. Innovations)"*. St. Petersburg, Saint Petersburg Electrotechnical University LETI, 2016, pp. 61–64.
2. Chistyakova T.B., Polosin A.N. Computer Modelling System of Industrial Extruders with Adjustable Configuration for Polymeric Film Quality Control. *Proceedings of 2017 IEEE II International Conference on Control in Technical Systems (CTS)*. St. Petersburg, Saint Petersburg Electrotechnical University LETI, 2017, pp. 47–50.
3. Shumyatskii Yu.I. *Promyshlennye adsorbtsionnye processy* [Industrial Adsorption Processes]. Moscow, KolosS, 2009.
4. Keltsev N.V. *Osnovy adsorbtsionnoy tekhniki* [Basics of Adsorption Technology]. Moscow, Khimiya, 1984.
5. Ruthven D.M., Farooq S., Knaebel K.S. *Pressure Swing Adsorption.* New York, Wiley, 1994.
6. Chin-Wen Wu, Vermula R., Kothare M., Sircar S. Experimental Study of a Novel Rapid Pressure-Swing Adsorption Based Medical Oxygen Concentrator: Effect of the Adsorbent Selectivity of N_2 over O_2. *Industrial & Engineering Chemistry Research*, 2016, vol. 55, no. 16, pp. 4676–4681.
7. Moran A., Talu O. Limitations of Portable Pressure Swing Adsorption Processes for Air Separation. *Industrial and Engineering Chemistry Research*, 2018, vol. 57, no. 35, pp. 11981–11987. DOI: 10.1021/acs.iecr.8b02237
8. Chai S.W., Kothare M.V., Sircar S. Rapid Pressure Swing Adsorption for Reduction of Bed Size Factor of a Medical Oxygen Concentrator. *Industrial and Engineering Chemistry Research*, 2011, vol. 50, pp. 8703–8710.
9. Akulinin E.I., Golubyatnikov O.O., Dvoretsky D.S., Dvoretsky S.I. Numerical Study of Cyclic Adsorption Processes of Air Oxygen Enrichment in Dynamics. *Journal of Physics: Conference Series*, 2019, vol. 1278, article ID: 012005.
10. Akulinin E.I., Golubyatnikov O.O., Dvoretsky D.S., Dvoretsky S.I. Optimizing Pressure-Swing Adsorption Processes and Installations for Gas Mixture Purification and Separation. *Chemical Engineering Transactions*, 2019, vol. 74, pp. 883–888.
11. Kirillin V.A., Sychev V.V., Sheindlin A.E. *Tekhnicheskaya termodinamika* [Technical Thermodynamics]. Moscow, MEI, 2016.
12. Dubinin M.M. *Adsorbtsiya i Poristost'* [Adsorption and Porosity]. Moscow, VAKhZ, 1972.
13. Akulinin E., Golubyatnikov O., Dvoretsky D., Dvoretsky S. Optimization and Analysis of Pressure Swing Adsorption Process for Oxygen Production from Air Under Uncertainty. *Chemical Industry and Chemical Engineering Quarterly*, 2020, vol. 26, no. 1, pp. 89–104.

14. Rice R.G., Do D.D. *Applied Mathematics and Modelling for Chemical Engineers*. New Jersey, Wiley, 2012.

15. Cruz P., Magalhaes F.D., Mendes A. On the Optimization of Cyclic Adsorption Separation Processes. *AIChE Journal*, 2005, vol. 51, pp. 1377–1395.

16. Kheifets L.I., Zelenko V.L., Pavlov Y.V. *Elementy teorii protsessov adsorbtsionnogo razdeleniya gazovykh smesey* [Elements of the Theory of Processes Adsorption Separation Gas Mixture]. Moscow, MGU, 2004.

17. Skvortsov S.A., Akulinin E.I., Golubyatnikov O.O., Dvoretsky D.S., Dvoretsky S.I. Mathematical Modelling of Cyclic Pressure Swing Adsorption Processes. *Journal of Physics: Conference Series*, 2018, vol. 1015, article ID: 032002. DOI: 10.1088/1742-6596/1015/3/032002

18. Goldstein A.L. *Optimizatsiya v srede MATLAB* [Optimization in MATLAB]. Perm, PNIPU, 2015.

Received November 25, 2019

УДК 661.935+519.633.2 **DOI: 10.14529/mmp200201**

ОПТИМАЛЬНОЕ ПРОЕКТИРОВАНИЕ ЦИКЛИЧЕСКОГО АДСОРБЦИОННОГО ПРОЦЕССА ОБОГАЩЕНИЯ ВОЗДУХА КИСЛОРОДОМ В УСЛОВИЯХ ЧАСТИЧНОЙ НЕОПРЕДЕЛЕННОСТИ

***Е.И. Акулинин*[1], *О.О. Голубятников*[1], *Д.С. Дворецкий*[1], *С.И. Дворецкий*[1]**
[1]Тамбовский государственный технический университет, г. Тамбов,
Российская Федерация

Сформулирована и решена задача оптимального (по критерию прибыли от производства кислорода) проектирования установки короткоцикловой безнагревной адсорбции (КБА) для обогащения воздуха кислородом в условиях частичной неопределенности исходных данных (состава, температуры, давления атмосферного воздуха) при наличии ограничений по чистоте кислорода, производительности установки и ресурсосбережению гранулированного адсорбента. Разработан эвристический итерационный алгоритм решения задачи оптимального проектирования в условиях частичной неопределенности исходных данных. Сформулирована вспомогательная задача оптимизации, относящаяся к классу задач нелинейного программирования (при допущении об аппроксимации непрерывных функций управлений на стадиях цикла «адсорбция-десорбция» step-функциями), решение которой осуществлялось методом последовательного квадратичного программирования. Поставленная задача оптимального проектирования была решена для типоряда установок КБА производительностью от 1 до 4 л/мин, позволяющих получать кислород с чистотой от 40 до 90 об.%. В ходе анализа полученных результатов установлены наиболее перспективные режимные и конструктивные параметры, обеспечивающие максимальную прибыль при функционировании установки КБА с учетом сбережения гранулированного адсорбента. Установлено, что введение ограничения на скорость газового потока в «лобовом» слое адсорбента установки КБА позволяет повысить надежность ее функционирования и увеличить срок службы адсорбента.

Ключевые слова: короткоцикловая безнагревная адсорбция; цеолит; математическое моделирование; оптимизация; проектирование; неопределенности.

Литература

1. Chistyakova, T.B. Joint Innovative IT Projects in the Field of Production of Polymeric Sheet Materials / T.B. Chistyakova, A.S. Razygrayev, A.N. Polosin, A.M. Araztaganova // Proceedings of the 2016 IEEE V Forum ≪Strategic Partnership of Universities and Enterprises of Hi-Tech Branches (Science. Education. Innovations)≫. – St. Petersburg: Saint Petersburg Electrotechnical University LETI, 2016. – P. 61–64.
2. Chistyakova, T.B. Computer Modelling System of Industrial Extruders with Adjustable Configuration for Polymeric Film Quality Control / T.B. Chistyakova, A.N. Polosin // Proceedings of 2017 IEEE II International Conference on Control in Technical Systems (CTS). – St. Petersburg: Saint Petersburg Electrotechnical University LETI, 2017. – P. 47–50.
3. Шумяцкий, Ю.И. Промышленные адсорбционные процессы / Ю.И. Шумяцкий. – М.: КолосС, 2009.
4. Кельцев, Н.В. Основы адсорбционной техники / Н.В. Кельцев. – М.: Химия, 1984.
5. Ruthven, D.M. Pressure Swing Adsorption / D.M. Ruthven, S. Farooq, K.S. Knaebel. – N.Y.: Wiley, 1994.
6. Chin-Wen Wu. Experimental Study of a Novel Rapid Pressure-Swing Adsorption Based Medical Oxygen Concentrator: Effect of the Adsorbent Selectivity of N2 over O2 / Chin-Wen Wu, R. Vermula, M. Kothare, S. Sircar // Industrial and Engineering Chemistry Research. – 2016. – V. 55, № 16. – P. 4676–4681.
7. Moran, A. Limitations of Portable Pressure Swing Adsorption Processes for Air Separation / A. Moran, O. Talu // Industrial and Engineering Chemistry Research. – 2018. – V. 57, № 35. – P. 11981–11987.
8. Chai, S.W. Rapid Pressure Swing Adsorption for Reduction of Bed Size Factor of a Medical Oxygen Concentrator / S.W. Chai, M.V. Kothare, S. Sircar // Industrial and Engineering Chemistry Research. – 2011. – V. 50. – P. 8703–8710.
9. Akulinin, E.I. Numerical Study of Cyclic Adsorption Processes of Air Oxygen Enrichment in Dynamics / E.I. Akulinin, O.O. Golubyatnikov, D.S. Dvoretsky, S.I. Dvoretsky // Journal of Physics: Conference Series. – 2019. – V. 1278. – Article ID: 012005.
10. Akulinin, E.I. Optimizing Pressure-Swing Adsorption Processes and Installations for Gas Mixture Purification and Separation / E.I. Akulinin, O.O. Golubyatnikov, D.S. Dvoretsky, S.I. Dvoretsky // Chemical Engineering Transactions. – 2019. – V. 74. – P. 883–888.
11. Кириллин, В.А. Техническая термодинамика / В.А. Кириллин, В.В. Сычев, А.Е. Шейндлин. – М.: МЭИ, 2016.
12. Дубинин, М.М. Адсорбция и пористость / М.М. Дубинин. – М.: ВАХЗ, 1972.
13. Akulinin, E. Optimization and Analysis of Pressure Swing Adsorption Process for Oxygen Production from Air Under Uncertainty / E. Akulinin, O. Golubyatnikov, D. Dvoretsky, S. Dvoretsky // Chemical Industry and Chemical Engineering Quarterly. – 2020. – V. 26, № 1. – P. 89–104.
14. Rice, R.G. Applied Mathematics and Modelling for Chemical Engineers / R.G. Rice, D.D. Do. – New Jersey: Wiley, 2012.
15. Cruz, P. On the Optimization of Cyclic Adsorption Separation Processes / P. Cruz, F.D. Magalhaes, A. Mendes // AIChE Journal. – 2005. – V. 51. – P. 1377–1395.
16. Хейфец, Л.И. Элементы теории процессов адсорбционного разделения газовых смесей / Л.И. Хейфец, В.Л. Зеленко, Ю.В. Павлов. – М.: МГУ, 2004.

17. Skvortsov, S.A. Mathematical Modelling of Cyclic Pressure Swing Adsorption Processes / S.A. Skvortsov, E.I. Akulinin, O.O. Golubyatnikov, D.S. Dvoretsky, S.I. Dvoretsky // Journal of Physics: Conference Series. – 2018. – V. 1015. – Article ID: 032002.
18. Гольдштейн, А.Л. Оптимизация в среде MATLAB / А.Л. Гольдштейн. – Пермь: ПНИПУ, 2015.

Евгений Игоревич Акулинин, кандидат технических наук, доцент кафедры «Технологии и оборудование пищевых и химических производств», Тамбовский государственный технический университет (г. Тамбов, Российская Федерация), akulinin-2006@yandex.ru.

Олег Олегович Голубятников, кандидат технических наук, старший преподаватель кафедры «Технологии и оборудование пищевых и химических производств», Тамбовский государственный технический университет (г. Тамбов, Российская Федерация), golubyatnikov_ol@mail.ru.

Дмитрий Станиславович Дворецкий, доктор технических наук, профессор, заведующий кафедрой «Технологии и оборудование пищевых и химических производств», Тамбовский государственный технический университет (г. Тамбов, Российская Федерация), dvoretsky@tambov.ru.

Станислав Иванович Дворецкий, доктор технических наук, профессор, профессор кафедры «Технологии и оборудование пищевых и химических производств», Тамбовский государственный технический университет (г. Тамбов, Российская Федерация), sdvoretsky@mail.tstu.ru.

Поступила в редакцию 25 ноября 2019 г.