MODELING AND ANALYSIS OF DYNAMICS OF PRESSURE SWING ADSORPTION PROCESS FOR SYNTHESIS GAS SEPARATION AND HYDROGEN PRODUCTION

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Abstract: On the basis of the Dubinin theory of micropore volume filling, a mathematical model of dynamics of pressure swing adsorption processes for synthesis gas separation has been developed. The model takes into consideration the influence of the processes of mass and heat transfer in gas and solid phases on the kinetics of diffusion transfer of adsorbate (carbon dioxide, carbon monoxide, hydrogen) in the adsorbent layer and accounts for all devices included in the process diagram (adsorber, compressor, vacuum pump, valves, throttle, receiver). Numerical studies of the process of separation of synthesis gas and concentration of hydrogen in a four-adsorber unit with granulated zeolite adsorbent 13X were carried out by methods of mathematical modeling: the influence of disturbing influences (composition and temperature of the initial hydrogen-containing gas mixture), regime parameters (cycle duration, pressure at the compressor outlet, pressure at the vacuum pump inlet, backflow coefficient) and design parameters (length of the adsorbent bulk layer and inner diameter of the adsorber) on the purity of the product hydrogen, its recovery rate and productivity of the unit were studied. The most dangerous disturbances and the most effective regime parameters of pressure swing adsorption process of synthesis gas separation were determined. It is established that the increase of temperature from 298 to 323 K and decrease of hydrogen concentration from 68 to 48 % (vol.) in initial gas mixture result in ~10 % lower efficiency of the unit due to the decrease of product hydrogen recovery rate. Practical recommendations on effective choice of operation regimes of an adsorption unit to ensure the achievement of required purity of product hydrogen at the level of 99.99 % (vol.), regardless of the impact of disturbances are formulated.

Nomenclature

a_k – sorption value of the primary adsorption layer, mole/m^3;

a^* – sorption value sorption value in equilibrium with the current concentration of adsorbate on the external granule surface in the flow, mole/m^3;

B – a parameter identifying the predominant size of adsorbent micropores, 1/K^2;

c_k – molar concentration of k-th component in gas phase, mole/m^3;

c_{pg} – specific heat capacity of the gas mixture, J/(mole·K);

D_g – effective longitudinal dispersion coefficient in the gas phase, m^2/s;

d_p – diameter of adsorbent granules, m;

n_k – index of power of the Dubinin equation;

h_k – sorption heat of k-th component, J/mole;

M_g – molar mass of gas phase, kg/mole;

S_{sp} – specific surface ration of adsorbent granules, m^2/m^3;

c_{pa} – specific heat capacity of the adsorbent, J/(kg·K);

$P_{s,k}$ – saturation pressure, atm;

$P_{m,k}$ – partial pressure, atm;

T_g – temperature of the gas phase, K;

T_a – temperature in the adsorbent, K;

W_0 – limiting adsorption volume, cm^3/g;

x – spatial coordinate of the length (height) of the adsorbent layer, m;

α – heat transfer coefficient from the surface of adsorbent granules to the gas mixture flow, referred to the phase interface unit, Wt/(K·m^2);

β_k – a kinetic coefficient of mass transfer of k-th component, 1/s;

υ_k^* – molar volume of k-th component, cm^3/mole;

λ_g – gas phase heat transfer coefficient, Wt/(m·K);

λ_a – adsorbent heat transfer coefficient, Wt/(m·K);

ε – adsorbent porosity coefficient, m^3/m^3;

v_g – gas flow velocity;

ρ_a – adsorbent density, kg/m^3;

ρ_g – molar density of the gas mixture, mole/m^3;

σ_k – affinity coefficient of k-th component to standard gas;

μ_g – dynamic viscosity of the gas phase, Pa·s;

ς – adsorbent granular sphericity factor;

τ – time, s

Introduction

Processes of pressure-swing adsorption (**PSA**) are widely used in industry for purification and separation of gas mixtures, concentration of various gases (hydrogen, oxygen, nitrogen, carbon dioxide, etc.). One of the urgent problems is the extraction of hydrogen from hydrogen-containing process flows (hydrocarbon conversion and oxidation gases, petroleum gases, synthesis gas, etc.) and its concentration up to 99.99 % (vol.). Typical substances accompanying hydrogen are carbon oxide and dioxide, nitrogen, methane, which have higher adsorption selectivity values [1]. Separation of synthesis gas and concentration of hydrogen is carried out in multi-adsorber PSA units using microporous adsorbents (granular active coals and zeolites of 5A, 13X with the highest capacity and selectivity for CO_2 and CO are most often used) [2 – 8].

In the process of operation of the PSA units there is a problem of ensuring the required technological indicators on the purity of the product hydrogen, its recovery rate and the unit productivity due to the influence of various disturbing influences. The sources of these are the instability of the composition and temperature of the initial gas mixture (synthesis gas), changes in the characteristics of the adsorbent during the

operation of the PSA unit, variations in the amount of the product flow bleed [9 – 12]. Thus, for example, synthesis gas obtained by Lurga method can contain approximately 15 – 18 % of CO, 38 – 40 % of H_2, 9 – 11 % of CH_4, 30 – 32 % of CO_2; the temperature of the initial gas mixture can vary from 20 to 50 ºC.

Mathematical modelling is a method recommended to study the effect of disturbing influences (composition and temperature of the initial hydrogen-containing gas mixture), regime parameters (cycle duration, pressure at the compressor outlet, pressure at the vacuum pump inlet, backflow coefficient) and design parameters (internal diameter of the adsorber, length and diameter of particles of the adsorbent bulk layer) on the recovery rate (concentration), purity of the concentrated hydrogen and productivity of the PSA unit [9, 10, 13 – 17].

In particular, in [18] Lopes et al. discuss mathematical modelling of a vacuum-pressure single adsorber PSA unit using granulated active coal as an adsorbent. The values of regime parameters (cycle duration and pressure at the balancing stage) providing hydrogen purity at the unit outlet more than 99.99 %, degree of its recovery 75 % and specific capacity of 160 mole H_2 per kg of adsorbent per day, were established.

In [19] mathematical modelling of hydrogen recovery process by steam methane reforming using PSA method was performed. It was established that pressure at adsorption stage, backflow coefficient and duration of adsorption stage influence the productivity of the unit, enabling to concentrate hydrogen with purity of more than 99.95 % and 80 % recovery rate. It is shown that increasing the concentration of hydrogen-related components in the initial gas mixture, in particular methane, leads to a decrease in purity of hydrogen at the outlet of the unit.

Tao et al. [8] have performed numerical studies of the pressure swing adsorption process of hydrogen concentration from five-component gas mixture carried out in a single-adsorber vacuum-pressure PSA unit. It was established that increasing the duration of the adsorption stage and the backflow coefficient leads to an increase in the purity of hydrogen and a decrease in the rate of its recovery.

The procedure of building a mathematical model of dynamics of pressure swing adsorption processes includes the following stages: 1) determining the structure of the model taking into account the effect of the transfer processes in all devices included in the process chart of the PSA unit (compressor, vacuum pump, valves, adsorbers, throttle, receiver, etc.); 2) obtaining experimental data on the PSA process under study, including the equilibrium conditions of adsorption and desorption processes of gas mixtures; 3) parametric synthesis of the model; 4) analysis and ensuring the adequacy of the mathematical model.

The aim of this research is to develop a mathematical model of dynamics of pressure swing adsorption process of synthesis gas separation and hydrogen concentration (using the theory of micropore volume filling of the Academician M.M. Dubinin) taking into account the influence of the processes of mass and heat transfer in the gas and solid phases on the kinetics of diffusion transport of adsorbate (H_2, CO_2, CO) in the adsorbent layer and the linkages of all devices included in the PSA unit. Also, numerical research of influence of regime and design parameters of the four-adsorber PSA unit for hydrogen concentration on purity of the product hydrogen, rate of its recovery and productivity of the unit within the specified range of changes of disturbing influences (composition and temperature of the initial hydrogen-containing mixture) will be conducted.

Mathematical description of dynamics of synthesis gas separation and hydrogen concentration process

The process of separation of synthesis gas and concentration of hydrogen up to 99.99 % (vol.) by the PSA method is carried out in a four-adsorber unit with granulated 13X adsorbent [20].

The pressure in the adsorbers is built up with the use of a compressor by opening controlled valves, through which the gas mixture to be separated is fed to the adsorbent layer. One complete unit operation cycle includes three stages: 1) adsorption mainly of CO_2, CO; in the adsorber the pressure is built up to the operating value, the product hydrogen is removed from the adsorbers and sent through the receiver to the consumer; 2) adsorption mainly of CO_2, CO (the adsorbent layer is regenerated by counter-current flow of the blow-off (hydrogen-enriched) gas mixture;) adsorption pressure reduction to atmospheric pressure; 3) pressure equalization in adsorbers (using the residual pressure in one adsorber after the adsorption stage to build up the pressure in another adsorber).

The following mass and heat exchange processes take place in the PSA unit during adsorption-desorption of H_2, CO_2 and CO with 13X zeolite adsorbent: a) diffusion of H_2, CO_2 and CO in the gas mixture flow; b) mass transfer of H_2, CO_2, CO and heat exchange between the gas phase and the adsorbent; c) adsorption of H_2, CO_2, CO on the surface and in micropores of zeolite adsorbent granules, with the evolution of heat; d) desorption of H_2, CO_2, CO from micropores and from the granule surface, with heat absorption.

In the mathematical description of the PSA process of synthesis gas separation and hydrogen concentration, the following assumptions were made: 1) the initial gas mixture (synthesis gas) is a three-component one (containing: $1 - H_2$ with concentration of $48 - 68$ % (vol.), $2 - CO_2$ with concentration of $27 - 47$ % (vol.), $3 - CO$ with concentration of 5 % (vol.)) and is considered as an ideal gas, which is feasible at pressures in the adsorber up to 200×10^5 Pa [21, 22]; 2) diffusion of H_2, CO_2, CO and heat distribution in the gas flow and granulated adsorbent is carried out in the longitudinal direction relative to the flow of the gas mixture in the adsorbent (by the height of the adsorbent layer) [18, 23 – 31]; 3) the process of adsorption-desorption of H_2, CO_2, CO by the adsorbent is carried out in the external diffusion area and is determined by the external mass transfer coefficient, the velocity of the gas mixture in the adsorbent layer, as well as the equilibrium relations of concentrations of H_2, CO_2 and CO in the phases [18, 24 – 26, 28, 30]; 4) granulated 13X zeolite with granule diameter 1.5 mm is used as adsorbent [2, 3, 32]; 5) adsorption equilibrium is described by Dubinin–Radushkevich equation [33]; 6) desorption branches of adsorption isotherms of H_2, CO_2, CO on 13X zeolite coincide with adsorption ones [1]; 7) gas temperature in receiver is equal to gas temperature at adsorption outlet, radiation heat loss is negligible.

In accordance with the accepted assumptions, the mathematical description of the processes occurring in the adsorber of the PSA unit during the separation of synthesis gas and hydrogen concentration includes the following equations:

1. Equations of component-wise material balance ($k = 1 - H_2$, $2 - CO_2$, $3 - CO$) in the gas phase flow by the adsorbent layer height [1]

$$\frac{\partial c_k(x,\tau)}{\partial \tau} + \frac{(1-\varepsilon)}{\varepsilon}\frac{\partial a_k(x,\tau)}{\partial \tau} + v_g(x,\tau)\frac{\partial(c_k(x,\tau))}{\partial x} = \frac{\partial}{\partial x}\left(D_g\frac{\partial(c_k(x,\tau))}{\partial x}\right), \qquad (1)$$

where $\varepsilon = 0.4$.

2. Sorption kinetics equation (Glueckauf equation) in a primary adsorption layer during internal diffusion transfer [33]

$$\frac{\partial a_k(x,\tau)}{\partial t} = \beta_k (a_k^* - a_k(x,\tau)), \qquad (2)$$

where a^* is determined by the sorption isotherm equation of Dubinin–Radushkevich [33]

$$a_k^* = \rho_a \frac{W_0}{\upsilon_k^*} \exp\left[-\left(\sqrt{B} \frac{T_g(x,\tau)}{\sigma_k} \lg\left(\frac{P_{s,k}}{P_{m,k}} \right) \right)^{n_k} \right], \qquad (3)$$

where $\rho_a = 2140$; $W_0 = 0.262$; $B = 2.2 \times 10^{-6}$; $\sigma_1 = 0.15$, $\sigma_2 = 2.31$, $\sigma_3 = 0.84$; $n_1 = 1$, $n_2 = 2$, $n_3 = 2$.

3. The equation describing the heat distribution in the gas mixture flow by the height of the adsorbent

$$c_{pg}\rho_g \frac{\partial T_g(x,\tau)}{\partial \tau} + c_{pg}\rho_g v_g \frac{\partial T_g(x,\tau)}{\partial x} - \frac{\alpha}{\varepsilon} S_{sp}\left[T_a(x,\tau) - T_g(x,\tau)\right] = \lambda_g \frac{\partial^2 T_g}{\partial x^2}, \qquad (4)$$

where $c_{pg} = 9971.44$; $S_{sp} = 4000$; $\lambda_g = 0.129$.

4. The equation of heat diffusion in the adsorbent

$$c_{pa}\rho_a \frac{\partial T_a(x,\tau)}{\partial \tau} + \alpha S_{sp}\left[T_a(x,\tau) - T_g(x,\tau)\right] - \sum_k h_k \frac{\partial a_k(x,\tau)}{\partial \tau} = \lambda_a \frac{\partial^2 T_a(x,\tau)}{\partial x^2}, \qquad (5)$$

where $c_{pa} = 830$; $\rho_a = 2140$; $\lambda_a = 0.139$.

5. Continuity and Ergun equations linking pressure and gas mixture velocity variations in adsorbent height [34]:

$$\sum_k c_k \frac{\partial v_g(x,\tau)}{\partial x} - v_g\left(\frac{\partial \sum_k c_k}{\partial x} \right) = 0, \qquad (6)$$

$$\frac{\partial P}{\partial x} = -\left(\frac{150(1-\varepsilon)^2}{(d_p\varsigma)^2 \varepsilon} \mu_g v_g + 1.75 M_g \rho_g \frac{(1-\varepsilon)}{d_p\varsigma\varepsilon^3} v_g^2 \right), \qquad (7)$$

where $\mu_g = 1.069 \times 10^{-5}$; $\varsigma = 1$.

Initial and boundary conditions for equations (1) – (7), formulas for calculation of parameters of mathematical model and adsorption equilibrium at separation of multicomponent gas mixture using Dubinin–Radushkevich equation, equation of pressure change in adsorbers and receiver of unit, flow rate of gas mixture passing through regulating inlet, outlet valves and throttle are presented in [35] and are not given here.

Thus, the mathematical description of the dynamics of the pressure swing adsorption process of synthesis gas separation and hydrogen concentration is a system of differential and finite equations, which is solved using the method of straight lines in the MATLAB software environment [36]. The accuracy analysis of the mathematical model was performed using the actual standard error between the model calculated and the experimental values of hydrogen purity at the adsorber outlet. The actual standard error was 0.15 % (vol.), which makes it possible to use the mathematical model for investigation of pressure swing adsorption processes and PSA units for synthesis gas separation and hydrogen concentration [9, 20].

When researching the effect of disturbing influences, regime and design parameters of the PSA unit on the performance indicators of the cyclic process

of hydrogen adsorption concentration the following were used: 1) as regime parameters of the PSA unit – the duration τ_{ads} of adsorption stage, which is equal to the stage of desorption τ_{des} and equalization τ_{eq} in terms of time period (in this case, the duration τ_c of the "adsorption-desorption" cycle is equal to $\tau_c = \tau_{ads} + \tau_{des} + 2\tau_{eq}$), the pressure P^{in} at the compressor outlet, the pressure P_{des}^{in} at the inlet of the vacuum pump; backflow coefficient θ, which determines the proportion of the product flow selected for adsorption regeneration; 2) as design parameters of the unit - length (height) L of the adsorbent bulk layer, internal diameter D of the adsorbent, diameter of particles d_p of the adsorbent bulk layer; 3) as disturbances - composition y^{in} and temperature T_g^{in} of the initial hydrogen-containing gas mixture supplied to the adsorbers for separation. Input data for computational experiments are presented in Table 1.

Based on the analysis of graphs of dependences of product hydrogen purity y_1^{out}, its recovery rate η and productivity of the unit G^{out} from the duration of adsorption stage τ_{ads} (at a nominal regime of PSA unit operation), duration of adsorption stage τ_{ads} can be set to 120 s (and, accordingly, cycle duration $\tau_c = 480$ s), at which hydrogen purity is reached at the level of $y_1^{out} = 99.99$ % (vol.) and maximum recovery rate is provided $\eta = 55$ % (Fig. 1).

An increase in the temperature of the initial gas mixture from 298 to 323 K leads to the need to reduce the duration of the adsorption stage τ_{ads} from 120 to 40 s due to a decrease in the equilibrium concentrations of carbon dioxide and carbon monoxide in the adsorbent (Fig. 2).

When the hydrogen content decreases from 68 to 48 % (vol.) and the carbon dioxide content in the initial gas mixture increases from 27 to 47 % (vol.), the adsorption capacity is exhausted faster, and the required hydrogen purity value at 99.99 % (vol.) is not reached (Fig. 3). Thus productivity of installation decreases on ~25 %. Calculations show that the increase of pressure at the compressor outlet from 17.5×10^5 to 23.5×10^5 Pa allows to increase productivity by ~25 %, but the rate of hydrogen recovery is reduced relative to the nominal regime from 55 % to 50 %.

Table 1

Source data for computational experiment

Variables	Variation range	Nominal value
Duration of the adsorption stage τ_{ads}, s	10…180	40
Pressure at the compressor outlet P^{in}, $\times 10^5$ Pa	5…30	17.5
Pressure at the inlet of the vacuum pump P_{des}^{in}, $\times 10^5$ Pa	0.5…1	0.75
Backflow coefficient θ, r.u.	1.25…15	5.83
Concentration of components in the initial mixture y^{in} $\qquad\qquad$ H$_2$ $\qquad\qquad$ CO$_2$ $\qquad\qquad$ CO	48…68 27…47 5	68 47 5
Temperature of the initial mixture T_g^{in}, K	293…323	298
Ratio of adsorber length to its diameter L/D	4…8	6
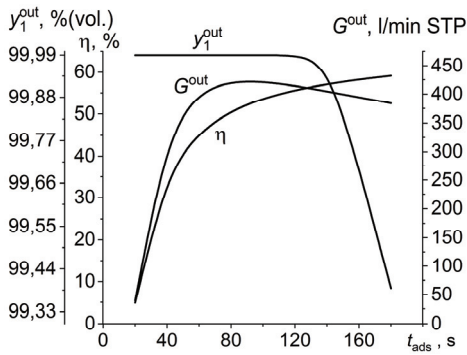
Fig. 1. Dependence of the purity of the product hydrogen y_1^{out}, its recovery rate η and the productivity of the unit G^{out} on the duration of the adsorption stage τ_{ads} at the nominal operating regime of the unit
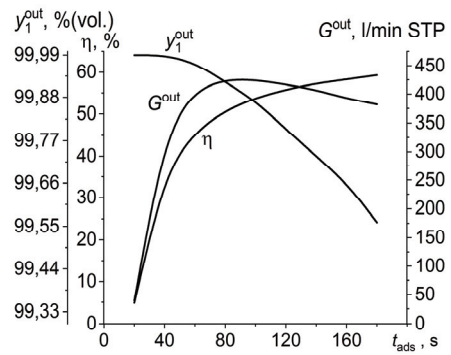
Fig. 2. Dependence of the purity of the product hydrogen y_1^{out}, its recovery rate η and the productivity of the unit G^{out} on the duration of the adsorption stage τ_{ads} at T_g^{in} = 323 K
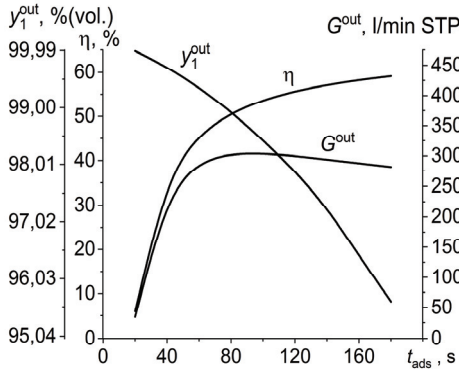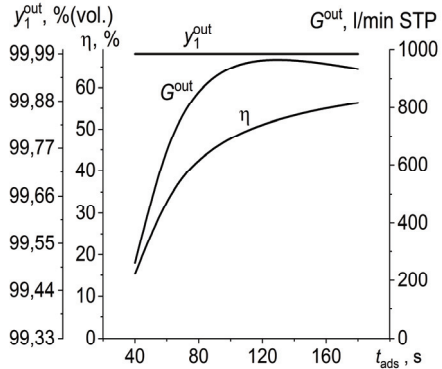
Fig. 3. Dependence of the purity of the product hydrogen y_1^{out}, its recovery rate η and the productivity of the unit G^{out} on the duration of the adsorption stage τ_{ads} at y_1^{in} = 48 % (vol.)

Fig. 4. Dependence of the purity of the product hydrogen y_1^{out}, its recovery rate η and the productivity of the unit G^{out} on the duration of the adsorption stage τ_{ads} at P^{in} = 30×10⁵ Pa

The increase in pressure at the inlet to the unit from 17.5×10^5 to 30×10^5 Pa leads to a decrease in the hydrogen recovery rate by ~10 % and an increase in productivity by 2.5 times (Fig. 4) relative to the nominal regime (Fig. 1). This fact is explained by an increase in the equilibrium concentration of recoverable components in the adsorbent when pressure P^{in} increases from 17.5×10^5 to 30×10^5 Pa. Decrease of pressure at an unit inlet from 17.5×10^5 to 5×10^5 Pa, on the contrary, leads to the increase of the hydrogen recovery rate by ~2 %, however productivity of the unit decreases by eight times (not shown in figures).

The increase in pressure at the vacuum pump inlet from 0.75×10^5 to 1×10^5 Pa leads to a reduction of adsorption stage duration from 120 to 50 s, the rate of hydrogen recovery from 55 to 48 % (not presented in figures). Decrease of pressure at vacuum pump outlet from 0.75×10^5 to 0.5×10^5 Pa increases the duration of adsorption stage

from 120 to 150 s, at which the required purity of product hydrogen $y_1^{out} = 99.99\%$ (vol.) is provided. The rate of hydrogen recovery decreases from 55 to 52 % due to an increase in the share of the flow taken for adsorbent regeneration. Calculations show that in order to increase the recovery rate up to 55 % (while maintaining hydrogen purity of 99.99 % (vol.)) in this regime it is necessary to reduce the backflow coefficient by ~5 % relative to its nominal value.

An increase in the length of the adsorbent bulk layer from 0.9 m to 1.2 m leads to a 5 % decrease in the recovery rate of hydrogen due to an increase in the pressure drop in the adsorbent layer (not shown in the figures). Decrease of adsorber length from 0.9 m to 0.6 m, on the contrary, results in the increase of hydrogen recovery rate on the average by 2 %, but the required level of hydrogen purity of 99.99 % (vol.) is not reached because of rapid depletion of adsorption capacity of adsorbent.

Conclusion

Using current methods of system analysis, mathematical modelling and computational experiments, new results have been obtained for the theory and practice of designing pressure swing adsorption processes of multi-component gas mixtures separation. The following parameters have been identified: 1) composition and temperature of the initial hydrogen-containing mixture have the most dangerous disturbing effects on the PSA process of synthesis gas separation and hydrogen concentration; 2) the most effective regime parameters are duration of the adsorption stage, pressure at the compressor outlet, pressure at the vacuum pump inlet and backflow coefficient. It is established that at increase of temperature from 298 to 323 K and decrease of hydrogen concentration from 68 to 48 % (vol.) in initial gas mixture, it is most expedient to increase pressure at compressor outlet by 1.7 times and lower backflow coefficient by ~5 % against their nominal values, but the efficiency of the unit will decrease by ~10 % because of the lower hydrogen recovery rate. It is also established that increase in length of adsorbent bulk layer from 0.9 m to 1.2 m causes increase in pressure drop in adsorbent layer and decrease in hydrogen recovery rate on the average by 5 %. Decrease in length of adsorbent bulk layer from 0.9 m to 0.6 leads to rapid depletion of adsorbent capacity and as a result the required purity of hydrogen of 99.99 % (vol.) cannot be achieved.

The mathematical model of the pressure swing adsorption process of synthesis gas separation can be used to study the dynamics of PSA processes of gas mixture separation, to optimize and improve the efficiency of PSA units with cyclically varying pressure.

The results obtained in this work can be applied to the design of new automated processes and pressure swing adsorption units for separation and purification of hydrogen-containing gas mixtures.

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Моделирование и исследование динамики адсорбционного разделения синтез-газа и концентрирования водорода

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Аннотация: На основе теории объемного заполнения микропор академика М. М. Дубинина разработана математическая модель динамики циклических адсорбционных процессов при разделении синтез-газа с учетом влияния процессов массо- и теплопереноса в газовой и твердой фазах на кинетику диффузионного переноса адсорбтива (диоксида углерода, монооксида углерода, водорода) в слое адсорбента и с учетом всех устройств, входящих в технологическую схему процесса (адсорбер, компрессор, вакуум-насос, клапаны, дроссель, ресивер). Методом математического моделирования проведены численные исследования процесса разделения синтез-газа и концентрирования водорода, осуществляемого в четырехадсорберной установке с гранулированным цеолитовым адсорбентом NaX: исследовано влияние возмущающих воздействий (состава и температуры исходной водородсодержащей газовой смеси), режимных (длительности цикла, давления на выходе компрессора, давления на входе вакуум-насоса, коэффициента обратного потока) и конструктивных параметров (длины насыпного слоя адсорбента и внутреннего диаметра адсорбера) на чистоту продуктового водорода, степень его извлечения и производительность установки. Определены наиболее опасные возмущающие воздействия и наиболее эффективные режимные параметры циклического адсорбционного процесса разделения синтез-газа. Установлено, что повышение температуры от 298 до 323 К и снижение концентрации водорода от 68 до 48 об.% в исходной газовой смеси приводит к снижению эффективности работы установки на ~10 % за счет уменьшения степени извлечения продуктового водорода. Сформулированы практические рекомендации по эффективному выбору режимов работы адсорбционной установки, обеспечивающие достижение требуемой чистоты продуктового водорода на уровне 99.99 об.% при воздействии возмущений.

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Simulation und Untersuchung der Dynamik der Adsorptionstrennung von Synthesegas und Wasserstoffkonzentration

Zusammenfassung: Basierend auf der Theorie der volumetrischen Füllung von Mikroporen des Akademiemitglieds M.M. Dubinin, ist ein mathematisches Modell der Dynamik zyklischer Adsorptionsprozesse bei der Trennung von Synthesegas entwickelt, das den Einfluss des Stoff- und Wärmeübergangs in der Gas- und Festphase auf die Kinetik des Diffusionsübergangs eines Adsorptionsmittels (Kohlendioxid, Kohlenmonoxid, Wasserstoff) in der Adsorbensschicht und unter Berücksichtigung aller im Prozessflussdiagramm enthaltenen Geräte (Adsorber, Kompressor, Vakuumpumpe, Ventile, Drossel, Auffänger) berücksichtigt. Numerische Untersuchungen des Prozesses der Trennung von Synthesegas und der Wasserstoffkonzentration in einer Vieradsorberanlage mit körnigem Zeolithadsorptionsmittel NaX sind unter Verwendung der Methode der mathematischen Modellierung durchgeführt: Einfluss der Störbeeinflussungen (Zusammensetzung und Temperatur des anfänglichen wasserstoffhaltigen Gasgemisches), Betrieb (Zyklusdauer, Drücke am Kompressorausgang und am Eingang der Vakuumpumpe, Rückflusskoeffizient) und Auslegungsparameter (Länge des Schüttbettes des Adsorbents und Innendurchmesser des Adsorbers) auf die Reinheit des Wasserstoffprodukts, den Extraktionsgrad und die Produktivität der Anlage durchgeführt. Es sind die gefährlichsten störenden Wirkungen und die effektivsten Betriebsparameter des zyklischen Adsorptionsprozesses der Synthesegasabtrennung bestimmt. Es ist festgestellt, dass ein Temperaturanstieg im Bereich von 298...323 K und eine Abnahme der Wasserstoffkonzentration von 68 auf 48 Vol.% im anfänglichen Gasgemisch zu einer Abnahme des Wirkungsgrades der Anlage um ~ 10% aufgrund einer Abnahme des Extraktionsgrades des Produktwasserstoffs führen. Für die effektive Auswahl der Betriebsarten der Adsorptionsanlage sind praktische Empfehlungen formuliert, die das Erreichen der erforderlichen Reinheit des Produktwasserstoffs in Höhe von 99,99 Vol.% unter dem Einfluss von Störungen sicherstellen.

Modélisation et étude de la dynamique de la separation par adsorption du gaz de synthèse et de la concentration en hydrogène

Résumé: A la base de la théorie du remplissage volumineux des micropores de l'académitien M. M. Doubinin est élaboré le modèle mathématique de la dynamique cyclique des processus de l'adsorption lors de la division du gaz de synthèse tenant compte de l'impact des processus de transfert de masse et de chaleur dans les phases gazeuse et le solide sur la cinétique du transfert de la diffusion de transfert de l'adsorbant (dioxyde de carbone, monoxyde de carbone, d'hydrogène) dans la couche d'adsorbant et compte tenu de tous les appareils entrant dans le schéma technologique du processus (adsorbant, compresseur, vide-pompe, vannes, clapet, réservoir). Par la méthode de la modélisation mathématique sont exécutées les études numériques du

processus de la séparation de gaz de synthèse et de la concentration de l'hydrogène dans une installation avec un adsorbant granulé zéolitique NaX: est étudiée l'influence des perturbateurs (composition et température du mélange), de régime (durée du cycle, pression de sortie du compresseur et l'entrée à vide de la pompe, coefficient d'inversion de l'écoulement) et les paramètres de conception (de la longueur de la couche de remplissement de l'adsorbant et du diamètre intérieur de l'adsorbant) sur la pureté de l'hydrogène, le degré d'extraction et la capacité de l'installation. Sont définis les effets perturbateurs les plus dangereux et les paramètres de fonctionnement les plus efficaces du processus d'adsorption cyclique de la séparation des gaz de synthèse Est constaté que l'augmentation de la température dans la plage de 298...323 K et la diminution de la concentration d'hydrogène de 68 à 48 vol.% dans le mélange de gaz entraîne une diminution de l'efficacité de l'installation d'environ 10% en réduisant le degré d'extraction de l'hydrogène. Sont formulées des recommandations pratiques pour un réglage efficace des modes de fonctionnement de l'installation d'adsorption, garantissant la pureté de l'hydrogène à 99.99 vol.% en cas de perturbations.

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