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МОДЕЛИРОВАНИЕ И АНАЛИЗ ПРОЦЕССА ХЕМОСОРБЦИИ ДИОКСИДА УГЛЕРОДА КАК ОБЪЕКТА УПРАВЛЕНИЯ

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В статье решены задачи моделирования процесса хемосорбции CO_2 и его анализа как объекта управления, а также приводятся рекомендации по синтезу структуры системы автоматического управления. На основе системного подхода сформулированы основные этапы и задачи анализа процесса хемосорбции как объекта управления. Решение поставленных задач приведено на примере пилотной установки насадочного абсорбера, в котором протекает процесс очистки газа от диоксида углерода раствором горячего поташа. Разработана математическая модель объекта, проведено исследование его статических характеристик, определены численные значения входных переменных и переменных состояния в статическом режиме. Математическая модель объекта построена исходя их допущений о секционной структуре абсорбера. Каждая секция представлена в виде ячейки идеального смешения по обеим фазам. Принято, что процесс хемосорбции протекает в диффузионно-кинетической области по реакции псевдо-первого порядка. Проведен анализ динамических характеристик объекта путем расчета реакции объекта на ступенчатое изменение входных переменных. Установлено, что объект не линеен по большинству динамических каналов. Синтезирована линеаризованная модель объекта в пространстве состояний, определены матрицы состояния и управления. Проведена оценка устойчивости стационарного состояния, наблюдаемости и управляемости объекта. Доказано, что объект обладает свойством устойчивости свободного движения. Для управления концентрацией CO_2 в выходном потоке газа предложено ограничиться результатами измерения только этой концентрации, а остальные компоненты вектора состояний оценивать с помощью наблюдателя. Даны рекомендации по структуре системы автоматического управления объектом.

Ключевые слова: хемосорбция, поташная очистка, системный анализ, моделирование, устойчивость, управляемость, наблюдаемость

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MODELLING AND ANALYSIS OF CARBON DIOXIDE CHEMISORPTION PROCESS AS OBJECT OF CONTROL

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In article problems of modeling of carbon dioxide chemisorption process and its analysis as object of control are solved. Also, the recommendations on synthesis of automatic control system structure are provided. Based on system approach the main stages and tasks are formulated for the analysis of process of carbon dioxide chemisorption by potash solution as object of control. The solution of objectives is given in the example of nozzle absorber pilot plant. The mathematical model of the object is developed, the research of its static and dynamic characteristics is conducted, variables of a state values are defined for given inputs. The mathematical model of the object is constructed on the basis of assumptions about the sectional structure of the absorber. Each section is presented as an ideal mixing cell for both phases. It is assumed that the chemisorption process proceeds in the diffusion-kinetic area through a pseudo-first order reaction. It is established that the object is not linear on most dynamic channels. The linearized object model in space of states is synthesized. Matrixes of a state and control are defined. The assessment of stability of steady state, observability and controllability of the object is carried out. It is proved that the object has property of stability of the free movement. It is controllable in the state of space and is observed when only carbon dioxide output concentrations measured. Recommendations on automatic control system structure for the object are offered.

Key words: chemisorption, potash purification, system analysis, modeling, stability, controllability, observability

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INTRODUCTION

Gas mixes purification from carbon dioxide in various industries is carried out by carbon dioxide chemisorption process realization, as a rule, in nozzle columns.

Use of a chemisorption is caused by insufficiently high solubility of carbon dioxide in water and leads to increase in driving force of absorption. In the industry a number of chemosorbent, such as monoethanol amine, diethanol amide, methyldiethanol amide, potassium hydroxide, a potassium carbonate, and others is applied [1-4].

Integrated approach to design of gases purification technological process and the corresponding control system assumes carrying out the system analysis of chemisorption process as object of control [5, 6]. The following tasks are solved:

- Analysis of technological process as a complex physical and chemical system and development of the mathematical description of object dynamics;
- Development of an algorithm and program for technological process computer modeling;
- A research of static and dynamic properties of model and transfer of results on an initial object;
- Analysis of steady state stability, observability and controllability, i.e. system-wide properties of an object.

The solution of these tasks is necessary in connection with continuous increase in requirements to quality and efficiency of functioning of the "absorbing column-control system" complex need to react flexibly to change of loading on a gas phase and the concentration of the absorbed component.

The literature analysis for this topic [1, 2] allows to draw a conclusion that, despite rather detailed description of the solution of the first two tasks, not enough attention is paid to the solution of the third and fourth tasks. Along with it, chemosorptionis coplex multistage process and is characterized by multidimensionality, nonlinearity and multiconnectivity [5, 7, 8] that causes complexity and not triviality of the specified tasks.

The dynamic mathematical model of chemosorption process in the columned plant generally represents system of the differential equations in private derivatives [9, 10] that complicates their application for synthesis of control systems. Therefore, the initial model with the distributed parameters is approximated by model with the concentrated parameters in the form of ordinary differential equations system [11]. The cell-like model which turns out from initial mathematical model by sampling of process on spatial coordinate [10] is most often used.

We will assume that dynamics of an object is described by model:

$$\begin{aligned}&\frac{d\bar{x}}{d\tau}=\bar{f}(\bar{x},\bar{u})\\&\bar{y}=C\cdot\bar{x},\end{aligned}\qquad(1)$$

where $\bar{x},\bar{u}$ n-dimention vector of state and r-dimenton vector of control, $\bar{y}$ m-dimensional vector of output variables, C – (m×n) measurements matrix, $\bar{f}(\cdot)$ – nonlinear functions and τ – current time.

The analysis of system-wide properties of an object with use of mathematical model in the form of (1) it is almost complicated [12]. Therefore for the solution of real tasks the equations, linearized in the neighborhood of model's steady state $\{\bar{x}^0,\bar{u}^0\}$ are used:

$$\begin{aligned}&\frac{d\hat{x}}{d\tau}=A\hat{x}+B\hat{u}\\&\hat{y}=C\cdot\hat{x},\end{aligned}\qquad(2)$$

where $A=\left\{\frac{\partial f_i}{\partial x_j}\right\}$, $i,j=\overline{1,n}$ state matrix, $B=\left\{\frac{\partial f_i}{\partial u_k}\right\}$, $i=\overline{1,n}$, $k=\overline{1,r}$ control matrix; $\hat{x}_i=x_i-x_i^{o}$; $\hat{u}_i=u_i-u_i^{o}$.

The control system consisting of an object and the actuation device can be efficient only in case own movements of system fade, i.e. the free movement of this system is steady. Information on object stability is a necessary for the algorithmic and parametrical synthesis of a control system.

According to the first method of Lyapunov [13], the studied object has property of stability of the free movement if roots of the characteristic equation det($\lambda_i I$-A) = 0, i.e. own numbers of a state matrix A λ_i, $i=\overline{1,n}$, have negative real-valued parts.

Proceeding from results of the object stability research, the task formulation for control system synthesis can be changed: in the case of steady object the paramount task is to ensure the required quality of control processes which are characterized by regulation time, with static and dynamic accuracy; in the case of unstable object problem definition for a control system synthesis comes down to ensure stability of the system free movement, and then to provide preset values of control processes quality indicators.

The necessary condition for realization of the object control system is controllability property of the object in a space of states. As not all classes of nonlinear objects allow receiving conditions of their controllability [12], in real tasks property of controllability is estimated by the analysis of the model (2) linearized in the neighborhood of a working point. At the same time, the assumption is used that if the linearized model is operated, then we operate also an initial nonlinear object.

To investigate the controllability of an object in a space of states the rank of controllability matrix is defined [9]:

$$У=\left[B\vdots AB\vdots A^2B\vdots\ldots\vdots A^{n-1}B\right].\qquad(3)$$

If the matrix (3) has a full rank, then an object has property of full controllability. For cases when there is an opportunity to organize various options of control vectors, it is necessary to carry out an assessment of the object controllability for various options of a matrix B in (2).

In practice, it is impossible to organize a complete measurement of a state vector; an important task is the research of the object observability. An object (2) has property of full observability if the observability

$$H=\left[C^T\vdots A^TC^T\vdots(A^T)^2C^T\vdots\ldots\vdots(A^T)^{n-1}C^T\right]\qquad(4)$$

has a full rank [9]. The structure of a matrix C, i.e. structure and quantity of the measured variables, has to provide a possibility to create the observer in case if it is impossible to measure full state vector.

MATHEMATICAL MODEL DEVELOPMENT

Object of control is the absorbing column consisting of three sections and filled with ceramic Rashig rings (Fig. 1). From above there are columns, in section 1, fresh absorbent – potash solution get in. The warmed-up to 100 °C, gas mix moves columns down – in section 3.

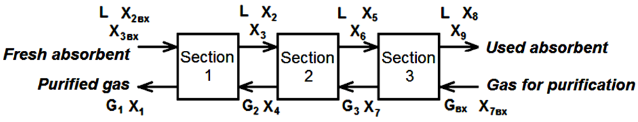

Fig. 1. The streams scheme in the partitioned absorber
Рис. 1. Схема потоков секционного абсорбера

In Fig.1 $x_{2вх}$ and $x_{3вх}$ – concentration of a potassium carbonate and potassium hydrocarbonate in an entrance stream of a chemisorbent, x_2, x_5, x_8 – concentration of potassium carbonate at output chemisorbent stream from 1, 2 and 3 sections, respectively, x_3, x_6, x_9 – concentration of potassium hydrocarbonate at the output of chemisorbent stream from 1, 2 and 3 sections, respectively, L – chemisorbent flow rate, $G_{вх}$ – input gas flow rate, $x_{7вх}$ – carbon dioxide concentration at the input gas stream, G_3, G_2, G_1 – output gas flow rate from 3, 2 и 1 sections, respectively, x_7, x_4, x_1 – carbon dioxide concentration at output of gas stream from 3, 2 and 1 cells respectively.

For the mathematical model development the assumptions are used that each section of an absorber represents a cell of ideal mixture on both phases, and, proceeding from chemisorption kinetics [14, 15], the process proceeds in diffusive and kinetic area on reaction of the pseudo-first order. The mathematical model consists of the equations of material balance for the absorbed substance in a gas phase and the equations of material balance for potassium carbonate and potassium hydrocarbonate in a liquid phase for each cell. The model describing dynamics of the top cell of the absorber at isothermal conditions is given below:

$$\frac{dx_1}{d\tau} = \frac{G_2 x_4}{V_1\varepsilon} - \left(\frac{G_1}{V_1\varepsilon} + B_1\right)\cdot x_1 + A_1\frac{x_3^2}{x_2}$$

$$\frac{dx_2}{d\tau} = L\frac{(x_2 - x_{2vx})}{V_1\delta} - B_2\cdot x_1 + A_2\frac{x_3^2}{x_2} \qquad (5)$$

$$\frac{dx_3}{d\tau} = L\frac{(x_3 - x_{3vx})}{V_1\delta} + 2\cdot B_2\cdot x_1 - 2\cdot A_2\cdot\frac{x_3^2}{x_2},$$

where V_1 – cell volume, ε – free volume share; δ – liquid holding ability, A_1, A_2, B_1, B_2 – the constant coefficients determined by a Henry's constant, reaction balance constant, reaction rate constant and mass transfer coefficient for a gas and liquid phases and also the regime parameters of technological process.

The full mathematical model of an object represents 9 equations of system describing dynamics of all three cells.

STEADY STATE AND DYNAMIC CHARACTERISITCS ANALYSIS

For a research of static and dynamic properties the modeling was held with Matlab Simulink of a package at the following technological, physical, chemical and kinetic parameters: absorber diameter – d = 0.052 m, l_1 = 1.66 m, l_2 = 0.96 m, l_3 = 1.10 m – nozzle layer height in cells 1, 2 and 3, respectively, ε = 0.7, δ = 0.1, L = =0.00041 m^3/min, $x_{2вх}$ = 1.53 kmol/m^3, $x_{3вх}$ = 0.77 kmol/m^3, $G_{вх}$ = 0.0086 m^3/min, $x_{7вх}$ = 0.033 kmol/m^3, specific surface of phases contact – a = 440 m^2/m^3, diffusion coefficient = $2.2\cdot 10^{-7}$ m^2/min, mass transfer coefficient in a gas phase K_g = 0.000033 kmol/m$^2\cdot$ min$\cdot$ kPa, mass transfer coefficient in the liquid phase, K_l = 0.003m/min, gas pressure P = 1080 kPa.

Steady-state and and dynamic characteristics of an object for the following channels are constructed: inputs →concentration of carbon dioxide at an output of gas stream, inputs →concentration of a carbonate of potassium and hydrocarbonate of potassium at an output stream of a chemisorbent.

In Fig. 2 and 3 the example of static and dynamic characteristics are presented *L*→x_1

Taking in consideration the static characteristics mode and comparison of object reaction to positive and negative step impacts, the conclusion can be made that an object is not linear on channels: input concentration of a carbonate of potassium – output variables, input flow rate of liquid absorbent – output variables and input gas pressure – output variables.

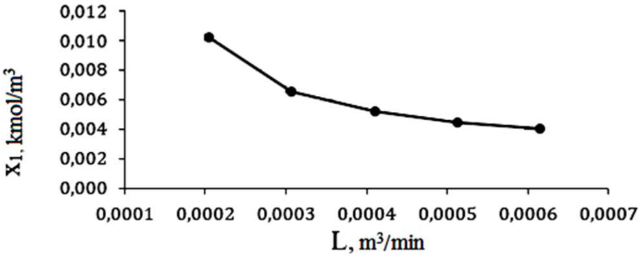

Fig. 2.Steady state characteristics on channel *L*→x_1

Рис. 2. Параметры устойчивого состояния по каналу *L*→x_1

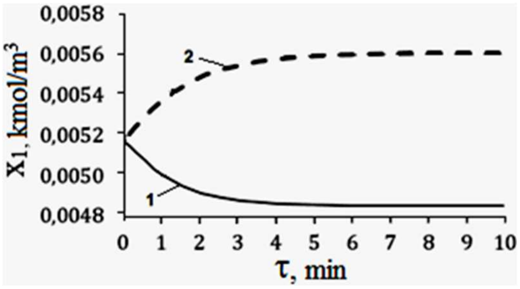

Fig. 3. Dynamic characteristics of an object on the channel *L*→x_1; 1 – at positive impact, 2 – at negative impact

Рис. 3. Динамические характеристики объекта по каналу *L*→x_1; 1 – при положительном воздействии, 2 – при отрицательно воздействии

OBJECT SYSTEM-WIDE PROPERTIES ANALYSIS

The next important task at a chemosorption research as object of control is studying its system-wide properties – stability of steady state, controllability and observability.

Proceeding from the purpose of functioning of an object the main objective of a control system is the stabilization of carbon dioxide concentration in an output of gas stream in the conditions of action of disturbances. As the control influence the input chemosorbent flow rate has been chosen: U = L.

Considering that the operated variable is output concentration of carbon dioxide in a gas stream at the exit of first cell, and the operating influence moves on an entrance of the first cell, it is expedient to investigate system-wide properties of an object by means of model of the first cell.

Passing in system of the equations (5) to variables increments $\hat{x}_i = x_i - x_i^{\,o}$, $i = \overline{1,3}$, $\hat{u} = u - u^{o}$, get the linearized object model (2).

State matrix A and roots of the characteristic equation det($\lambda_i I$-A) = 0 have the following values:

$$A = \begin{pmatrix} -8.832 & -0.005627 & 0.01239 \\ -40.13 & -1.203 & 0.08781 \\ 80.26 & 0.07977 & -1.339 \end{pmatrix}; \quad \lambda_i = \begin{pmatrix} -8.9923 \\ -1.1632 \\ -1.2186 \end{pmatrix}$$

As all own numbers are negative and various, the studied object has property of stability of the free movement.

The research of observability property allows to formulate a task for development of the system of measurement proceeding from tasks for automatic control system. In case of impossibility of all condition parameters measurement realization, the structure and the number of the measured parameters of a state have to provide a possibility of observer creation.

The following options of practical measuring system realization have been evaluated:

- all condition variables x_1, x_2, x_3 are measured,
- only x_1, x_2 are measured,
- only x_1, x_3 are measured,
- only x_1 is measured.

The observability matrix (4) analysis shows that the matrix has a full rank $rank(H) = 3$ in all cases. This means that the object is fully observed in different cases of the state parameters measurements.

For the controllability evaluation, the controllability matrix has been designed. The task is to analyze the controllability during the stabilization of carbon dioxide concentration system development with chemisorbent flow rate as a control parameter $U = L$.

$$У = \begin{pmatrix} 0 & -12.923 & 131.954 \\ 425 & -585.913 & 1.326 \cdot 10^3 \\ -850 & 1.172 \cdot 10^3 & -2.653 \cdot 10^3 \end{pmatrix}$$

It is established that the matrix has a full rank $rank(У) = 3$, that says that an object is characterized by property of full controllability.

CONCLUSION

In the article the research of nozzle absorber pilot plant, in which purification process of gas from carbon dioxide is realized with solution of hot potash as object of control, modeling of an object and a research of its properties is carried out.

It is established that the free movement of an object in the neighborhood of a working point is asymptotically steady that confirms property of stabilizability of an object. Main results of the research of object system-wide properties, and its static and dynamic characteristics allow to state possible options of problem definition for automatic control system design.

Todesignthecarbondioxidecontrolsystem-inoutgasflowwiththeliquidflowasacontrolparameter U=L the measuring of x_1 will be enough other components of state vector can be evaluated with the observer.

The control algorithm and method of parametrical synthesis should be chosen taking into account the fact that an object is nonlinear on most dynamic channels. One of ways to solve this problem is the application of methods of the synergetic control theory [16].

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