Modeling and Optimization of Adsorption Processes

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***Abstract*— The work is dedicated to the development of scientific principles of optimal design of the adsorption of binary and three-component liquid and gaseous mixtures in industrial sorbents.**

***Keywords*— adsorptive; 3-component system; modeling; optimization**

I. Introduction

The proportion of the use of adsorption processes in refining and petrochemical industries grows systematically in the modern world. The reasons is that the processes of adsorption (clean from the environmental point of view), prevent pollution. Their economic indicators are also high in comparison with other processes [1].

The systematic analysis of different sorbents, especially sorption processes involving industrial sorbents ,carried out. some of the issues including - thermal effects, the research process in the transitional regime, the concentration and temperature profiles of binary and three-component systems, the dependence of the diffusion coefficient on concentration and temperature of the adsorptive, as well as on the rate of flow of raw materials, the adsorption at high pressure and variable values , stagnant zones of industrial adsorbers, etc., separation by adsorption of aromatic and paraffinic hydrocarbons, sulfur compounds from gasoline fractions, as well as gas mixtures has not been studied [2].

In many industrial applications adsorbernyh separation of the components, in general, involves several steps (adsorption, desorption, the return of the waste after the heating and cooling of the sorbent for reuse), and these stages, along with other parameters, are characterized by a kind of time. Identification of the relationship property stagnation zones and time of accession one canister to another is of great scientific and practical importance, both for the improvement of existing adsorbers, and for a preliminary determination of experimental parameters of the designed adsorbers.

The above noted shows the relevance of creating a mathematical model that gives the best opportunity to manage the process of adsorption of binary and three-component liquid and gaseous mixtures.

II. Statement of the Problem

To achieve this goal required in a systematic way the implementation of the following research:

- determine the stability of binary patterns (*n*-oktan/*n*-geksadekan, *i*-oktan/n-geksadekan, *n*-oktan / benzene (toluene) and 3-component system (aromatics / paraffinic hydrocarbons / organic compounds of sulfur)– transient concentration and temperature profiles, the process of drying the sorbent under various conditions:
- determine patterns of change in effective diffusion coefficients and overall mass transfer, depending on the elucidation of 3-component gas mixtures and the amount of absorbed substances at high pressures on the length of the adsorbent layer, the definition of zones of high mass transfer and protection from the study macrokinetics multicomponent gas system;
- construction of a mathematical model of the process of adsorption of a mixture of liquid and gaseous mixtures, and on its basis in a transient condition, the implementation of the optimal design and control of adsorption processes.

III. Solution of the Problem

First found in industrial adsorbents adsorption characteristics of binary (n-oktan/n-geksadekan, i-oktan/n-geksadekan n-oktan / benzene (toluene) and 3-component (aromatics paraffins hydrocarbons / sulfur-containing organic compounds) systems with time-dependent concentration profiles of the condition, temperature, velocity, and transient patterns of existing and planned industrial adsorbers. As a result, a comprehensive study of unsteady areas of stagnant zones adsorbers, a mathematical expression for the dependence of these areas of concentration, temperature and flow rate of raw material and it is added to the general mathematical model of the process, developed the method of calculating the values of diffusion coefficients and the scientific basis for adaptive optimal control of industrial adsorption plants.

The results of the pilot study developed a method for calculating the values of diffusion coefficients, depending on concentration, temperature and flow rate of the adsorptive material. This dependence is shown in the form of mathematical equations and added to the general mathematical model. As a result of scientific bases of adaptive optimal control of industrial adsorption plants.

There was built a mathematical model of the process of adsorption of a fixed bed of adsorbent in transient conditions. The mathematical expression of mass transfer coefficient β on various parameters has been empirically compiled. Revealed that the condition $\frac{D}{d_{gr}} \geq 30$ (here, *D*-diameter of the adsorber; d_{qr} is diameter of grain of the adsorbent) for adsorption process of multicomponent mass transfer is increased sufficiently [3].

On a 4-adsorption plants operating in continuous mode for the adsorption process, liquid paraffins, found the optimal values of the transition time from one stage to another. The duration of the stages of adsorption and desorption were similar. The optimal value of this time was equal to 6.34 hours. Also, the duration of the stages of drying and cooling, respectively, is equal to 6.29 and 6.32 hour. The optimal value of the full cycle of adsorption was equal to 25.29 hours. As a result of optimization in a fixed bed adsorber to be resistant form hydraulic regime. In this state, the flow rate is constant and the concentration at all points distributed evenly. In consequence of this inside the canister between the ablative and the separation sections can prevent the formation of stagnant zones.

These results, in terms of optimal design of an industrial plant of 4 adsorbers (full cycle adsorption separation - 28 hours) are of great practical importance.

IV. Conclusion

As a result of scientific and comprehensive study, the adsorption of a gas mixture of methane, nitrogen and CO 2 revealed that in a state of optimal design developed during the formation of the adsorption equilibrium in the absorber is reduced by 25 seconds and 70 seconds. Therefore, taking into account the stagnation zone in the adsorber, mass transfer is significantly improved [4].

As the result of the work it was found that the unused portion of the length of the adsorption layer, (if you do not take into account the stagnant zone) is 5.8% of the total length of the fixed bed of adsorbent, and is equal to 1.2%.

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