

REPUBLIC OF AZERBAIJAN

On the rights of the manuscript

ABSTRACT

of the dissertation for the degree of Doctor of Philosophy

**ISSUES OF OPERATIONAL PROCESS MANAGEMENT
OF HYDROCARBON DEHYDROGENATION ON THE BASIS
OF A COMPUTER SYSTEM OF SIMULATION IN REAL
TIME**

Specialty: 3337.01 Information - measuring and control system
(in the chemical industry)

Field of science: Technical sciences

Applicant: **Nubar Alimurad Guliyeva**

Baku -2024

The work was performed at Sumgait State University, Automation and Control department.

Scientific supervisor: doctor of technical sciences, professor
Ali Hesen oglu Nagiyev

Official opponents: doctor of technical sciences, professor
Gambar Agaverdi Guluyev

doctor of technical sciences, professor
Azer Kahraman Mammadov

Ph.D. in technology, associate professor
Afag Tofiq Mammadova

Dissertation council ED 2.04 of the Supreme Attestation Commission under the President of Republic of Azerbaijan operating at Azerbaijan Technical University

Chairman of the Dissertation council: doctor of technical sciences, professor
Nurali Adil Yusifbayli

Scientific secretary of the Dissertation council: Ph.D. in technology, associate professor
Vahid Gara Farhadov

Chairman of the scientific seminar: doctor of technical sciences, associate professor
Mazahir Muhammad Isayev

GENERAL CHARACTERISTICS OF WORK

Relevance and development of the topic. Hydrocarbon dehydrogenation processes using fluidized bed technology of fine-grained catalysts are the main method for producing lower and partially middle alkenes, which are raw materials for the production of various polymers. These processes are carried out in technologically complex reactor-regenerator units, which are characterized by the presence of a catalyst mass circulation system between the reactor and the regenerator. The specific features of these processes as objects of operational control are caused by a number of properties emanating mainly from the inseparable connection of two reaction apparatuses, characterized by the presence of both direct and feedback connections.

As a result of the catalytic dehydrogenation process, coke is formed, which can clog the channels in the porous structure of the catalyst particles. Consequently, the catalyst loses activity very quickly during the residence time of the particles in the reactor. This is the reason for the circulation reduction of the catalyst, which is carried out by burning out the coke accumulated in the pores of the catalyst, where, along with the latter, the actual raw materials and reaction products are also adsorbed at a temperature of $T = 650-670$ 0C. The heat generated in combustion constitutes the main part in the thermal balance of the system; even modes are acceptable when the process turns out to be self-sufficient in thermal terms, i.e. without introducing additional fuel into the regenerator.

Obviously, the rates of reactions, including coke deposition reactions, have an Arrhenius dependence on temperature, therefore, a kind of dynamic connection is created between the chemical processes in the reactor and the thermal processes in the regenerator. This connection aggravates the control processes - small changes in any device can lead to large disturbances, up to an emergency increase or decrease in temperature in the system.

From all of the above, the peculiarity of this process as an object of control was born. The simple approach of observing the specified values of the mode parameters in the “regulations” does not at all solve the control problem. The fact is that there are “strong” disturbances: - from changes in the plant’s loading of raw materials, the degree of coke content of raw materials, thermal combustion processes (non-burnout of coke, i.e. the CO:CO₂ ratio during combustion depends on many factors), etc. d.

Consequently, the processes in the reactor and regenerator cannot be considered separately. A holistic approach is needed - the model must cover both the processes of coke formation and combustion, which occur in different apparatuses that have a dynamic connection with each other.

The traditional approach currently used in the world practice of industrial production, which consists in the desire to improve the stabilization of individual operating parameters at a given level, does not completely solve the problem, although the need for the presence of the latter is also not excluded.

Considering this feature of the object, the relevance of the problem is quite obvious, which consists in the development of appropriate control technology in a wide range of changes in state variables, which can be based on the creation of a unified, at the same time nonlinear, mathematical model for controlling the thermal regime of the entire system.

Object and subject of the research. Chemical-technological processes that are carried out in a fluidized bed of a pulverulent catalyst with its continuous regeneration are considered. Unlike dehydrogenation processes, which are carried out in the system of cyclic recovery of catalyst activity, in this technology, the processes proceed in a continuous flow of raw materials to the plant, and it is distinctive that in this design the catalyst is circulated in the reactor-regenerator system. An example is the processing of butane, isobutane, isopentane.

Aims and objectives of the research. The aim of the study is to develop a mathematical model of the dynamics of the thermal states

of the reactor-regenerator unit, which carries out the processes of hydrocarbon dehydrogenation, which can serve as the basis for indirect real-time measurement of the depth of catalyst coking at the outlets of two corresponding apparatuses, i.e. reactor and regenerator. The use of a detailed mathematical description of the dynamics of the processes taking place in the system should serve as solutions to control problems in a wide range of state variables and provide local control by negative feedback.

Research methods. The study applied methodologies for constructing mathematical models of controlled dynamic systems based on the theory of differential equations, chemical kinetics, control theory and stability theory, methods for identifying dynamic systems and real-time simulation techniques.

The main provisions defended:

1. Mathematical structure of the kinetic model of the reactor-regenerator block of the hydrocarbon dehydrogenation process.

2. Statement of the problem of indirect measurement of catalyst coking in the processes of catalytic dehydrogenation of hydrocarbons in a fluidized catalyst bed.

3. The method of parametric identification of the mathematical model of the dynamics of the thermal states of the reactor-regenerator unit, based on the introduction of mismatches, separately both for static states and for the dynamics of transient modes.

4. Real-time control algorithms based on a nonlinear mathematical model of complex dynamic systems.

Scientific innovations of research. The scientific innovations of the dissertation consist of the following:

1. Mathematical structure of the thermal nonlinear model for controlling the dynamic states of the reactor-regenerator block of the hydrocarbon dehydrogenation process.

2. Method for indirect measurement of physically non-measurable coordinates of a non-linear dynamic system in real time using signals from a part of the measurable coordinates of the hydrocarbon dehydrogenation process.

3. Construction of a model of coke deposits in the pores of the catalyst based on the fractal representation of the chaotic structure of a highly porous finely dispersed catalyst.

4. Two-criteria problem of parametric identification of the thermal model of the reactor-regenerator block of the hydrocarbon dehydrogenation unit, based on the formation of a package of testing pulses.

5. Dimension reduction of the reactor-regenerator dynamic system in the process of hydrocarbon dehydrogenation based on automatic stabilization of one coordinate of the state vector.

6. Statement and solution of the control problem for large deviations of the thermal coordinates of the reactor block of hydrocarbon dehydrogenation units.

Theoretical and practical significance of research. For the first time, a mathematical model of a system including processes of coke deposition on a catalyst has been obtained in relation to the process of dehydrogenation of isobutane to isobutylene. The mathematical model of this process and related algorithms for real-time control of the processes in the light of state monitoring and control in a wide range of state variables can be applied in the process control modes on similar reactor-regeneration systems with a fluidized bed of a catalyst.

Approval and application. The main provisions of the dissertation were discussed at the following conferences: Republican scientific conference dedicated to the 90th anniversary of Academician Togrul Shakhtakhtinsky, Baku 2015; Proceedings of the International Scientific and Technical Conference dedicated to the day of the Chemist and the 40th anniversary of the Department of Chemical and Technological Processes of the branch of the Ufa State Petroleum Technological University in Salavat, UFA, 2017; XXI Republican Scientific Conference of Doctoral Students and Young Researchers, Baku, 2017; International Scientific Conference, Sumgayit, 2018; International Scientific Conference Information Systems and Technologies of Achievements and Prospects, Sumgayit,

2020; IV Republican Scientific Conference Applied Problems of Mathematics and New Information Systems, Sumgayit, 2021.

The name of the institution where the dissertation work was performed. Dissertation work was performed at the Department of Process Automation of Sumgayit State University.

The total volume of the dissertation is indicated by noting the volume of the structural sections of the dissertation separately. The dissertation was written in accordance with the requirements set by the Higher Attestation Commission under the President of the Republic of Azerbaijan. Dissertation title page 421 conventional mark number, table of contents 7245 conventional index number, introduction 5699 conventional index number, consists of four chapters, conclusion, bibliography and appendices. The main content of the work consists of 147 pages, 17 pictures, 24 graphs and 3 tables. 106 sources are listed in the bibliography. Dissertation consists of 204084 characters without tables, figures and bibliography.

MAIN CONTENTS OF THE WORK

The introduction provides a rationale for the relevance of the research topic, comments on the purpose and tasks to be solved, questions submitted for defense, lists the novelty of scientific results and their practical significance.

The first chapter is devoted to the chemical essence of the processes of hydrocarbon dehydrogenation and a review of literature sources in the field of modeling and controlling these processes, in particular, the process of isobutane dehydrogenation in a fluidized catalyst bed.

Features of technological schemes for the implementation of catalytic processes for the dehydrogenation of hydrocarbons in a fluidized bed. Analysis of literary sources for solving management problems.

Catalytic dehydrogenation of hydrocarbons (DOH) is one of the brightest representatives of the class of technologies used to implement chemical processes in reactor-regenerator systems. Based

on the fact that the contact of hydrocarbon feedstock with a fine-grained catalyst (or a pulverized one) is the most optimal, it is necessary to apply the technology of organizing the fluidization mode (FB) of the catalyst, both in the reactor and in the regenerator. A sufficiently high feedstock conversion rate is fraught with rapid coking of the catalyst and a decrease in its activity, which necessitates its parallel purification by oxidative regeneration. Both the contact of the catalyst with the feedstock and with air in the parallel process of oxidative coke removal occur in the FB, which can only be organized in the catalyst circulation system between the reactor and the regenerator. This is the main feature of these systems, since it is it that causes many problems of monitoring and controlling the thermal regimes of the "reactor-regenerator" unit. It can be noted with certain confidence that the design, complicated by the indicated technological feature, which manifests itself in the problems of controlling the processes of hydrocarbon dehydrogenation, has a number of specific aspects. Figure 1 shows one of the widely used designs for the dehydrogenation of alkanes (butane, isobutylene, isopentane). Here, the catalyst is transported to the apparatuses in identical U-shaped pipes, from the reactor with air, and back with nitrogen.

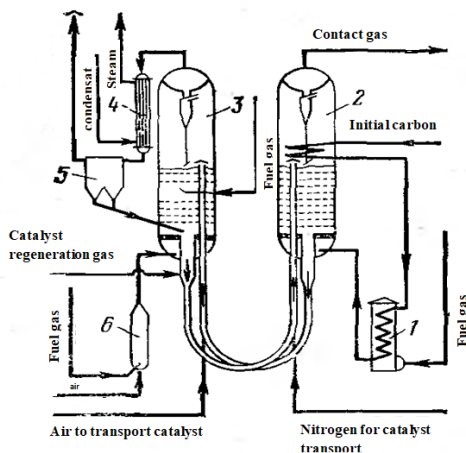


Figure 1. Plant for dehydrogenation of alkanes with U-shaped transport lines

Note that in this study, some aspects of the engineering solution in this design are taken into account when modeling the reactor-regenerator system.

The technical difficulties associated with the complexity of the technological scheme, first of all, include the solution of the problem of automatic control. The fact is that one of the important technological measurements, which is the operational control of the degree of coking of the catalyst, is a technically difficult problem to solve. The average residence time of the catalyst in the reaction apparatus is on the order of 10-16 minutes, during which the assessment of the state of the catalyst should be carried out without any perceptible delay.

Obviously, this problem can be solved only with the use of in-line measuring instruments, the creation of which remains problematic to this day due to the high temperature and aggressive environment.

In this regard, attention is drawn to some efforts to involve stochastic methods of information processing, such as kinetic data of reactions (including the oxidation of coke deposits). Most authors, in order to solve the problem of stabilizing the thermal states of the RR system, pose the problem of robust control of the tuning parameters of a linear automatic temperature control system. In a number of cases, this task is reduced to the development of a Kalman filtration system, only to avoid the need for detailed kinetic studies of the coke formation process.

In the scientific and technical literature, the issues of mode stabilization based on PID control are covered. In these systems, the PLC and the SCADA system are often found as the central elements of the technical solution.

Concerning the topic of control visualization, the practice of using programmable logic controllers (PLC) in industrial automation should be emphasized. These tools have recently been especially developed in the field of visualization in the dynamics of the flow of the control process in real time. The compactness of designs, which contributes to their release in the form of built-in elements, creates favorable conditions for access to operational information and the

implementation of control commands. Due to the significant reduction in the PLC response time to external signals, it has now become possible to successfully use it in control with visualization of the control process itself.

Works in the field of mathematical modeling of closed chemical systems reactor-regenerator suitable for control in a wide range of state variables. Among the first works concerning modeling in circulating reactor-regenerator systems, there is work of Cairo University professor S.S. Elnashaie. From the point of view of creating the foundations of a systematic approach to studying the regularities of the dynamics of thermal regimes of reactor-regenerator units, we note that the contribution of this and a number of subsequent works of this researcher deserves special attention.

The kinetics of hydrocarbon dehydrogenation processes has been studied in detail by domestic chemists. In the field of control engineering, the ideas of combining heat and material flows in a single system of differential equations turned out to be fundamental, the foundations of which were laid in the works of the 70s by the now Academician of ANAS A.M. Alieva² with employees. Modeling of thermal dynamic states of RRB is reflected in the works of A.G. Nagiev and co-authors. In these works, dynamic nonlinear models of both the reactor and the regenerator are developed for the process of catalytic cracking of heavy oil residues. The widespread use of the kinetic mechanisms of combustion of coke deposits is the influence of the above-mentioned works that favored the creation of an extended structure of the dynamic model of the RRB. Later works in this area raised the question mainly regarding the identification of the dependences of output indicators on regime parameters.

In this regard, it is important to note that in this work, in order to model the dynamics of the RRB in the PS, it was strategically planned to give preference to a pseudo-homogeneous representation of the PS structure.

The use of a statistical approach to describing the state of the reaction catalytic system instead of a phenomenological one, i.e. outside the consideration of the laws of motion of a single catalyst

particle, it turns out to be justified and expedient. weight of the catalyst.

As regards the processes of hydrocarbon dehydrogenation, it should be emphasized that a feature of these processes is the high sensitivity of the catalytic effect to the state of chromium in the structure of the catalyst matrix. Studies of dehydrogenation processes are dominated by works devoted to the study of the effect of the valence of chromium in the composition of the catalyst.

There are attempts to carry out parametric identification of the model of coke formation on the basis of a number of laboratory analyses.

It should be noted that a special direction in the field of mathematical modeling is the so-called cybernetic approaches, which is characterized by the predominance of the informational aspect in modeling. From this point of view, the use of fuzzy logic in modeling and creating situational control attracts attention. Fuzzy logic turns out to be effective for describing the probability of occurrence of critical situations leading to violations in the fluidized bed regimes in the regenerator.

Thus, as a result, attention should be paid to a number of aspects of the analysis.

1. As a generalization of the design options for reactor-regenerator blocks for the implementation of the dehydrogenation of hydrocarbons with a microspherical catalyst, in particular, isobutane, it is advisable to focus on the structural model of U-type installations of transport lines (Fig. 2). This model, in contrast to the other models mentioned, for example, the Ortoflow model, which is more often used for catalytic cracking of heavy hydrocarbons, or the 1A-1M model, which is also used for these processes, is in good agreement with the main modern requirements. These requirements are mainly reduced to the reliability of the circulation of the catalyst, ease of control of the mode of the thermal system, as well as the convenience of influencing the degree of residual coke on the surface of the regenerated catalyst.

2. Measurement of the degree of coking of the catalyst, both at the outlet of the reactor after the implementation of the actual chemical

process in a fluidized bed, and after regeneration, encounters a technical problem, which consists in the practical impossibility of creating measuring instruments for establishing in flows. The main reason is the abrasive effect of the flow, the presence of high temperature and the influence of the resinous environment. Accurate model estimation of the coking depth of the catalyst is a significant contribution to the solution of the present problem.

3. The category of a mathematical model can be a kinetic form in the form of a system of differential equations built on the basis of balances of coke formation rates and the kinetic regularity of the chemical reaction of a high-temperature oxidative process in the presence of atmospheric oxygen.

4. Mathematical modeling of a really functioning industrial system can be successful only if it is based on parametric identification according to the data of a specific industrial installation. Any obstacles associated with conducting active experiments to obtain information for solving the problem of parametric identification can be eliminated by using adaptive real-time tuning in the operating mode of a technically ready system.

MATHEMATICAL MODELING OF THE PROCESS.

Generalized RRB scheme, classification of basic coordinates

The processes of catalytic dehydrogenation of hydrocarbons can be structurally represented as a closed catalyst circulation system between the reactor, where the target chemical transformations are actually carried out, and the regenerator, which acts as an activity restorer by removing coke deposits on the catalyst (Fig. 2). Moreover, the concept of “recovery” includes, in addition to the removal of coke deposits, also the restoration of the valence of chromium in the composition of the catalyst, since the catalyst, entering the regenerator in a high temperature environment, undergoes oxidative transformation of catalytically active 6-valent chromium into inactive 3-x valent chromium.

For mathematical modeling for the purposes of management, a necessary step is the classification of variables according to their role in the management process. Let's make the following classification:

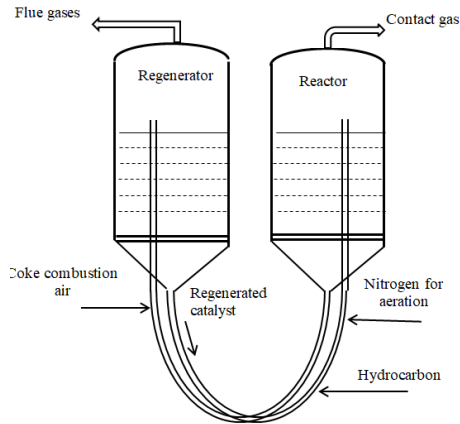


Figure 2. A simplified flow diagram of the relationship between the reactor and the regenerator in terms of material flows and the main coordinates of the system

1. Input coordinates. This should include both parameters that change independently of the operating personnel - disturbances, and control, which is in the introduction of the governing body, in particular: - the consumption of raw materials for the installation, the so-called. coke content of a batch of raw materials; - control parameters - catalyst circulation rate in the system, - input of additional fuel for heating the regenerator, - nitrogen consumption for aeration in the transport line for introducing raw materials into the reactor.

2. Coordinates of the state space.

The model of the dynamics of thermal states can be quite fully represented by four coordinates: - the temperature of the reactor and regenerator and the degree of coking of the catalyst at the outlets of the reactor and regenerator.

If the on-line temperature measurement in apparatuses does not encounter any difficulties, then the on-line measurement of the other two coordinates is one of the tasks of close attention in this work.

A special section of this work is devoted to the issue related to the problems of physical measurement of this parameter, therefore, we will limit ourselves here only to the fact that at present there is no physical measuring device for performing operational control of this coordinate.

It is important to note that the listed coordinates are the space that defines the thermal state, and the extended state space has a dimension equal to eight. We mean two additional coordinates - these are the concentrations of trivalent chromium at the outlets of two reaction apparatuses.

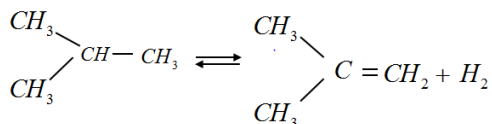
3. Output coordinates.

The output coordinates in this formulation of the research problem can be not only one, but also different parameters, which are somehow associated with the state coordinates. For example, one of the options may be the yield of the target product.

Obviously, within the framework of this study, the main attention is directed to the problem of controlling the state coordinates, i.e. the second item of this list, in fact, has a direct purpose and is oriented towards mathematical modeling of precisely dynamic processes in the reactor-regenerator unit.

Kinetic description of catalyst coking on the example of isobutane dehydrogenation.

Let us dwell on one of the examples - the example of the dehydrogenation of isobutane to isobutylene. The production of isobutylene from isobutane proceeds according to the following scheme:



It is important to note that, along with the target reaction, side reactions also occur, among which we will focus on coke formation reactions. Coke is a combination of heavy hydrocarbons and coal itself, with an average weight ratio C:H = 12-19.

Omitting the formal records of the system of differential equations, which are given in the dissertation to describe the kinetics of the reactions of the formation of coke deposits, we restrict ourselves to the following formal representation:

$$w_k = F_1(\bar{k}_k, T_1, \nu)$$

where \bar{k}_k – generalized rate coefficient of coke formation reactions, T_1 – temperature in the reaction zone; ν – the mass rate of input of raw materials into the reactor, which in this interpretation is taken as equivalent to the generalized concentration of coke-forming reactions.

It is expedient to present the formal notation of the rate equation for the coke burning reaction in the form:

$$\nu = F_2(k_2, T_2, f_\theta, \nu_z)$$

where $\nu, k_2, T_2, f_\theta, \nu_z$ – respectively, the mass rate of the catalyst regeneration reaction, the generalized rate constant, the regenerator temperature, the air flow into the regenerator, and the fuel gas flow into the coke combustion zone.

To take into account the reversible transitions of trivalent and hexavalent chromium in the process of catalyst regeneration, we will compose a kinetic record of the reactions of chromium valence change in the following form:

$$\frac{dC_{Cr^{6+}}^{(2)}}{d\tau} = k_{+3} \exp(-E_2 / RT_2) C_{Cr^{6+}};$$

$$\frac{dC_{Cr^{3+}}^{(1)}}{d\tau} = k_{+6} \exp(-E_1 / RT_1) (1 - C_{Cr^{6+}}^{(1)}) C_{2,3};$$

where $C_{Cr^{3+}}^{(1)}, C_{Cr^{6+}}^{(2)}$ – concentrations of trivalent and hexavalent chromium in the regenerator, k_{+3}, k_{+6} – coefficients, rates of corresponding reactions; E_1, E_2 – activation energies of the fall

reaction and recovery of catalyst activity, R – universal gas constant, τ – time.

Development of a unified thermal model of RRB based on material and heat balances

Creating a single (holistic) mathematical model, we used an approach based on the description of the feedback mechanism through the main RRB channels:

$$\begin{aligned}
 G_1 \frac{dC_1}{dt} &= F_k(C_2 - C_1) - \phi_1(T_1, C_1, C_2, w)G_1; \\
 G_2 \frac{dC_2}{dt} &= F_k(C_1 - C_2) + \phi_2(T_2, C_2)G_2; \\
 G_1 c_k \frac{dT_1}{dt} &= F_k c_k (T_2 - T_1) - \phi_1(T_1, C_2, w)q_2 G_1 + \\
 &\quad + c_{raw} F_{raw} (T_{raw} - T_1) + k_{en} S_1 (T_{en} - T_1); \\
 G_2 c_k \frac{dT_2}{dt} &= F_k c_k (T_1 - T_2) + \phi_1(T_2, C_1)q_1 G_2 + q_3 F_{fu} + \\
 &\quad + q_4 \delta F_k + F_{air} c_{air} (T_{air} - T_2) + k_{en} S_2 (T_{en} - T_2);
 \end{aligned} \tag{1}$$

where C_1, C_2, T_1, T_2 – coke concentration and temperature in the reactor and regenerator; F_k, F_{air}, F_{raw} – catalyst mass flow rates, air into the regenerator and raw materials into the reactor; $k_{en}, S_1, S_2, G_1, G_2$ – coefficient of heat transfer to the environment, areas of contact with the environment of the reactor and regenerator, the mass of the catalyst in the corresponding apparatuses; c_k, c_{raw}, c_{air} – heat capacity of the catalyst, raw materials and air, $\phi_1(T_1, C_2, w)$, $\phi_2(T_2, C_2)$ functions for describing kinetic factors based on the Arrhenius form.

The presented structure of the mathematical model of the dynamics of the thermal regime of RRS is based on a quasi-homogeneous representation of the reaction medium of the catalyst fluidized bed without separate consideration of the oxidation reactions of coke deposited on the surface and in the pores inside the catalyst. This important aspect was taken into account with the introduction of

the so-called "pseudo channel" design, which includes an appropriate accounting factor. The latter concept is based on the fractal analysis of the porous structure of the catalyst. Below, this concept will be described in relation to modeling the process of deep coke removal in catalyst pores.

Note that in (1) the functions of the rates of coke formation and recovery of catalyst activity are approximated by the following expressions:

$$\begin{aligned} \phi_1(T_1, C_1, C_2 w) &= k_{01} \exp(-E_1 / RT_1) \frac{\alpha w C_1}{1 + \exp(-\beta C_2)}; \\ \phi_2(T_2, C_2) &= k_{02} \exp(-E_2 / RT_2) C_2^\eta; \eta = 1.0 - 1.4 \end{aligned} \quad (2)$$

where w – weight rate of input of raw materials, α, β, η – constant numbers.

Fractal description of coking processes on the catalyst surface

The fractal analysis of stochastic geometric structures in this study is taken as the basis for modeling the processes of both coke deposition and oxidative reduction of catalyst activity. The use of this method was carried out in combination with the description of the processes of molecular diffusion in macro, meso - and micro channels of a porous medium.

In this regard, the hypothetical structure known in the literature as the dendritic model of the pore system of a solid material turned out to be very effective. Using this hypothetical, geometric construction and based on the abstract “pseudo-channel” model, a formulation was made to calculate some mass transfer coefficients deep into the porous material. The following formulas are used to estimate the effective mass transfer coefficients of a substance.

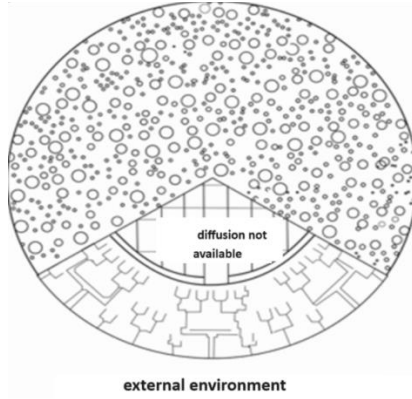


Figure 3. Dendritic structures in a grain of a porous catalyst and a core inaccessible to diffusion

Total perimeters $\Pi'(\ell)$, cross-sectional area $S'(\ell)$ and volume of branches with length equal $V'(\ell)$, according to the geometry of the cylindrical channel and taking into account the relationship $r = b\ell$ can be calculated as follows:

$$\Pi'(\ell) = \frac{2\pi\ell}{b} \left(\frac{\ell_0}{\ell} \right)^{D_{\Pi}} \quad (3)$$

$$S'(\ell) = \frac{\pi\ell^2}{b} \left(\frac{\ell_0}{\ell} \right)^{D_S} \quad (4)$$

$$V'(\ell) = \frac{\pi\ell^3}{b^2} \left(\frac{\ell_0}{\ell} \right)^{D_V} \quad (5)$$

where D_{Π}, D_S, D_V - fractal dimensions, based on parameters

$a = \frac{r_{n+1}}{r_n} = \frac{\ell_{n+1}}{\ell_n}$, $\frac{r_n}{\ell_n} = b$, $\frac{\chi_{n+1}}{\chi_n} = c$ are calculated by expressions:

$$D_V = 3 + \frac{\ln c}{\ln a}; D_S = 2 + \frac{\ln c}{\ln a}; D_{\Pi} = 1 + \frac{\ln c}{\ln a}, \quad \text{where } r_n, \ell_n -$$

radius, length of the cylindrical channel; χ_n - the number of branches

in the dendrite trunk; n – generation number in the dendritic formation.

Relations (3)–(5) can serve as a measure of diffusion drag, which is known to be a function of channel sizes. In other words, the greater the restriction for volumetric or surface molecular diffusion, the more noticeable the drop in the rate of oxygen delivery deep into the channel for the combustion reaction.

Mathematical model for simulating the dynamics of processes during fuel heating of the regenerator.

In the control process, there are situations in which it is necessary to introduce an additional amount of gas fuel into the regenerator. A situation is created in which not only the hydrodynamic situation changes, but also the regime with an oxygen deficiency manifests itself, despite the fact that in a normal situation it is its excess that takes place. This situation requires a revision of the structure of the mathematical notation of combustion processes, already taking into account the existence of two phases - a dense one, where catalyst particles create a uniform (concentrated) phase, and a rarefied one, which is the result of air bubbles due to a higher air flow rate.

The third chapter is devoted to the study of the static and dynamic properties of reactor-regenerator unit models based on the characteristics of the isobutane dehydrogenation process. into account the processes of heat and mass transfer between these two phases:

Parametric identification of a mathematical model according to industrial plant data.

In the field of parametric identification of industrial reactor-regenerator systems, there is a positive experience regarding the technology of the catalytic cracking process. This is based on the so-called principle of testing influences. The idea of the principle is that the mismatch function can be constructed from the statistics of equilibrium (mostly statistical) states, adding to these empirical data some experimentally obtained transient regimes. Borrowing this concept, taking into account the technological features of the system under consideration, turns out to be as successful as the systems previously used in the literature. The mismatch function in relation to our model takes the following form:

$$R(p_1, p_2) = \sum_{i=1}^4 \sum_{j=1}^{N_1} \left(y_{ij}^M(p_1, p_2, u_j) - \xi_{ij}^T \right)^2 + \alpha \cdot \sum_{i=1}^4 \sum_{n=1}^{N_2} \left[Y_i^M(p_2, u_n, t_n) - Y^T(t_n) \right]^2 \rightarrow \min \quad (6)$$

where $p_1 \in P_1; p_2 \in P_2$ – vectors of identifying parameters to be determined; y_{ij}^M, Y_i^M – respectively, the components of the 4-dimensional state vector of the system (1) and the vector during forced movement after the test pulse; ξ_{ij}^T – experimental values of statistical data, N_1 – the number of observations (stationary regimes that make up the actual statistics); indices M, T – the values calculated from the equations and the experimental values, respectively; t_n – discrete time step, α – criterion weight coefficient with respect to transient dynamic states. Note that the equations of stationarity states are obtained in the form of the right-hand sides of differential equations (1) and static dependences (2) equated to zero.

The identification of the parameters of the static states of equations (1) is suitable for ordinary passive statistics, when the so-called package of testing transient modes should include a certain number of acceleration characteristics for certain channels. One of the components of this package is shown in Fig. 4.

When minimizing the function (6), it is provided for the variable parameters p_1, p_2 and α to change the level of preference due to the weight coefficient α , because the second component of the residual function (6) is aimed at the mismatch in dynamics.

Obtaining transfer functions according to the model (1), (2) through the channels involved in the problem of local mode stabilization

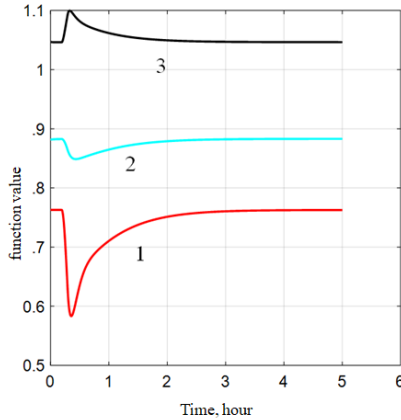
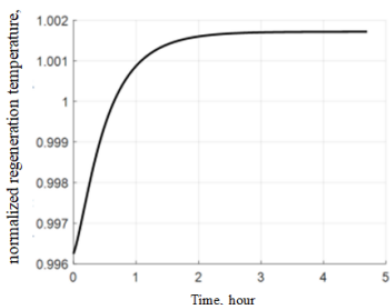


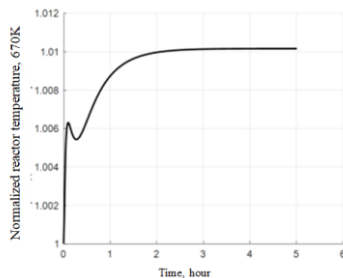
Figure 4. The reaction of the system to an impulse decrease in the speed of the catalyst: 1- degree of coking after regeneration; 2- reactor temperature; 3- regenerator temperature

As you know, the technology for creating linear stabilization systems in industry is based on the methodology of transfer functions, which in turn are based on the Laplace transform. Obviously, the presence of a dynamic model of the system in the form (1), (2) frees one from the troublesome operation of obtaining acceleration curves on a real object, replacing it with a 5% “step” at the inputs. The paper provides calculations for the linearization of the dynamic model along arbitrarily given channels.

On fig. 5 (curves a, b) shows the transient processes of establishing a new steady state after a stepwise decrease in the rate of air input into the regenerator with a swing of 5% ($F_{raw}(t_0) = 1.15 \cdot F_{raw}^{nom}$) and system response (in terms of temperature) to a 15% step change in the feed rate into the reactor ($F_{raw}(t_0) = 1.15 \cdot F_{raw}^{nom}$). As can be seen, within 1.2-14 hours, the system acquires the main part of the new regeneration temperature value, and then the increase in this state variable is not noticeable.



a)



b)

Figure 5. Change in the temperature of the regenerator (a) and reactor (b) after a 5% decrease in the volumetric velocity of air supplied to regeneration

The fourth chapter is devoted to the development of algorithms for solving the problem of monitoring and managing the thermal regime of RRBs based on a nonlinear mathematical model of the system.

Rapid assessment of the degree of catalyst coking using model (1), (2).

In connection with this task, a schematic diagram of an indirect measurement system based on a dynamic model has been developed.

The principle underlying this system is to synchronize the solution of a system of differential equations with the phase trajectories of a real industrial facility. Synchronization is supposed to be carried out according to temperature coordinates that are involved in the hardware environment of the information support of the proposed automated control system. The values of catalyst coking should be determined indirectly, i.e. by the values of the two corresponding components of the phase coordinate vector.

Obviously, with this approach to the problem of estimating the values of physically impossible measurements, the main problems arise, the synchronization of the above two forced movements - “object-model”.

are performed on the basis of "model-object" simulation, it is not difficult to come to the conclusion that the main source of error is the error of the RRB model and the duration of the period between the two basic laboratory by analysis.

Therefore, the closer in time the act of measurement is to the moment of setting the initial conditions of the basket for the start of the system, the more the model-object desynchronization errors are eliminated. Therefore, the formula that takes into account this source of error is expressed as

$$\Delta Z(\eta, \tau) = \Delta Y \pm \varphi(\eta, \tau); \tau = t - t_{start}; \varphi = e^{\alpha\eta\tau}$$

Where ΔY – object model error; τ – respectively, the time with the beginning of the countdown from the moment of the start of the "measurement mode" ($t - t_{start}$); t_{start} – moment of achieving synchronization «model-object», α – approximation coefficient; η – signal-to-noise ratio along the input vector.

The figure shows the time diagram of the change in time of the accuracy of the virtual control.

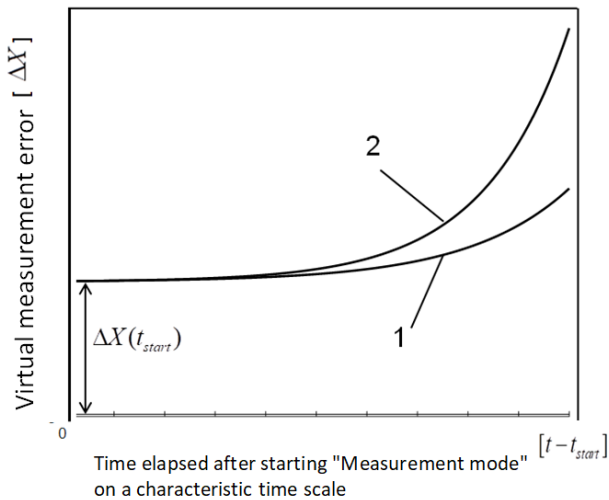


Figure 7. The nature of the influence of “model-object” desynchronization on the accuracy of virtual measurement

In conclusion, we note that due to the high inertia of industrial control processes in RRB and the not so high level of “signal-to-noise”, as well as the presence of laboratory analysis standards in production, the described virtual measurement algorithm can be taken as a completely acceptable method for operational monitoring of the state of a controlled object .

Reducing the order of the system of differential equations (1), (2) by stabilizing the temperature in the reactor through external influences, which are not included in the above equation, serves an important purpose - creating visual representations of the dynamics of the process. Modern information technologies aimed at facilitating the functioning of human-machine systems are increasingly being developed, convincingly demonstrating the rationality of using visualization tools in real-time control processes.

Achieving a sufficient level of stability in time of one of the coordinates of the reactor-regenerator unit will allow us to consider a family of trajectories in the phase space of the projection of three coordinates. Obviously, posing and solving such a question is associated with a rather serious task, since the temperature in the reaction zone is influenced by a large number of operating factors. This includes the consumption of raw materials for processing, the heating temperature of the raw materials, and the main effect is the influence of the thermal regime of catalyst regeneration. Therefore, this problem can be successfully solved only if a reliable channel for influencing this coordinate is found for the thermal system. We drew attention to the existence of a technological line for introducing nitrogen into the transport line (Fig. 8a).

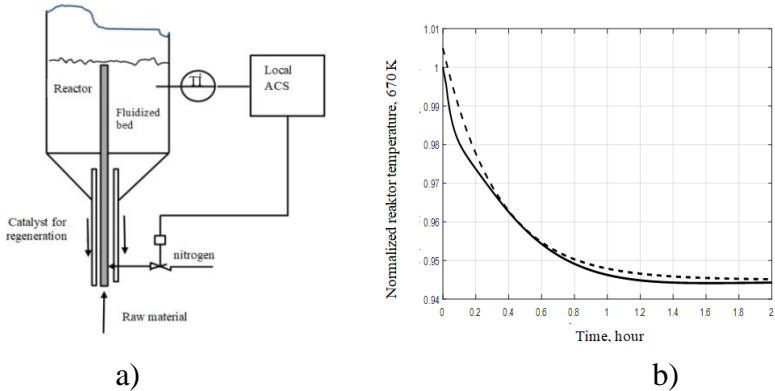


Figure 8. Principal diagram of temperature control system with influence on the nitrogen consumption in the transport line and the response of system (1), (2) to the stepwise perturbation from the side of increasing nitrogen input into the reactor transport line (solid curve) and its approximation (dashed curve)

Possessing a fairly significant transmission coefficient, this channel is completely isolated from other state variables and controls.

In Fig. 9. a block diagram of the feedback path for stabilizing the reactor temperature is shown.

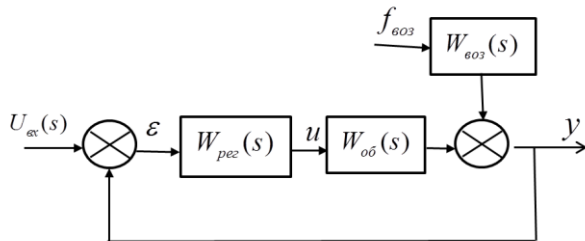


Figure 9. Block diagram of the feedback path in the reactor temperature stabilization system

The dedicated inputs correspond to the task for the stabilized temperature value and the disturbance that is applied at the point of feedback action. For both of these channels, it is of interest to study the reactions of the system with feedback.

When choosing a regulatory law, we proceeded from the consideration “from simple to complex.” Those. assumed that in this context, any complication could lead to additional clutter, resulting in an unjustified complexity of visualization of the result.

According to the structural diagram, based on the Laplace transform, we write:

$$u(s) = \left(K + \frac{1}{T_u s} \right) \varepsilon(s) ; W_p(s) = \left(K + \frac{1}{T_u s} \right)$$

Let us write down the equation for the transmission of a single step along the channel "U_{ex} - y":

$$G_z(s) = \frac{W_p(s)W_{o\delta}(s)}{1+W_p(s)W_{o\delta}(s)}$$

where

$$\begin{aligned} W_{ob}(s) \cdot W_p(s) &= W_0(s) = \left(\frac{k}{T^2 s^2 + 2T\xi s + 1} \right) \left(K \cdot s + \frac{1}{T_u s} \right) = \\ &= \frac{KkT_u s + k}{T^2 T_u s^3 + 2T\xi T_u s^2 + T_u s} . \end{aligned}$$

Figure 10 below shows the control channel transition processes in four options. The indicated options correspond to the following values of the parameters of the proportional-integral controller:

1. $K = 2.55; T_u = 200;$
2. $K = 1,24; T_u = 300;$
3. $K = 0.85; T_u = 600;$
4. $K = 0,9; T_u = 100.$

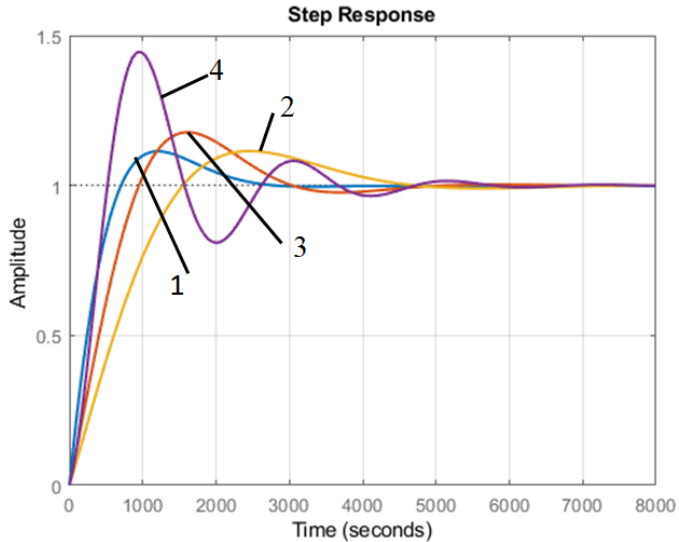


Figure 10. Transition process of the closed system on the control channel

As it can be seen, the use of an integrating resistor in the feedback circuit could not prevent the transition process from being oscillating in general. However, it is possible to obtain more suitable switching processes as a result of selecting the appropriate tuning parameters in the PI control system.

Development of local control systems for state variables using programmable logic controllers

In this section, the focus is shifted to the direction of the interconnectedness of the state vector of the system (1), (2) and to the issue of ensuring the controllability of the remaining coordinates when providing control actions within the framework of the ACS of a given coordinate.

The limited channels of influence on the object can manifest themselves negatively in this very issue. Therefore, generally speaking, the question of stabilization of state variables in general for all coordinates can have its correct solution only under the conditions of direct measurements of all state variables. In this case, it is necessary to use multi-connected automatic control systems with

transfer functions of all cross communication channels and the presence of a vector of control actions with sufficient dimension.

In the absence of these capabilities, still, if certain requirements are met, the task of stabilizing one of the coordinates of the system under consideration can be set, including in the feedback circuit one of the indirectly estimated coordinates, in particular, the residual coking of the catalyst after regeneration. On the other hand, it should be taken into account that when feedback covers one coordinate, it is necessary to control overruns beyond the established boundaries of other coordinates.

Note that these features of the control problem are very successfully solved by means of programmable logic controllers.

Creation of a local system for stabilizing residual catalyst coking based on a programmable logic controller of the SIMATIC series

Solving the issue of indirectly measuring the degree of catalyst purity after regeneration creates real conditions for creating closed control circuits for a number of variable reaction-regeneration systems, i.e. ACS of temperatures in the reactor and regenerator, degree of coking of the catalyst at the outlet of the reactor and regenerator.

Note that these technological variables are subject to a rather strong influence from the catalyst circulation rate, and at the same time, the number of independent channels influencing the phase coordinates is not so large. Here we are obviously talking about technological variables covered by feedback loops.

As for the software tools for performing calculations for establishing tuning parameters and ensuring the required quality and stability of the synthesized system, both in the Simulink system (Matlab application) and in the Simatic programming system from Siemens there are sufficient modules for the corresponding purpose. The only difference is that the software library of these controllers does not contain a block for implementing transfer functions necessary for simulating and constructing control systems other than a single-loop

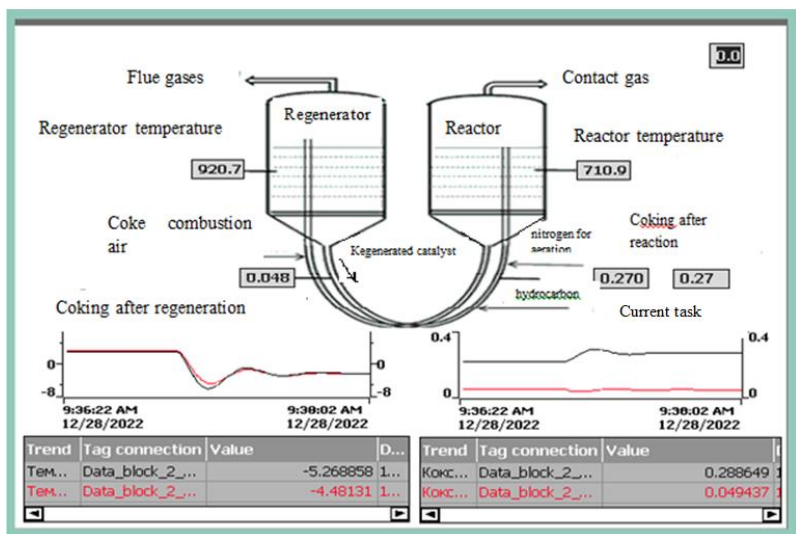


Figure 11. Screen (Screen) for visualization, which allows real-time execution of the function of monitoring the measured parameters, both in digital and graphical form, as well as changing the setting of the controller of the selected parameter of the controlled parameter

As for the software tools for performing calculations to establish the tuning parameters and issues of ensuring the required quality and stability of the synthesized system, then, as in the Simulink system (Matlab application) and in the Simatic programming system from Siemens, there are sufficient modules for the appropriate purpose. The only difference is that in the software library of these controllers there is no block for implementing the transfer functions necessary for simulating and building control systems other than a single-loop scheme. This issue was solved by the method proposed by a group of employees¹ of the Department of

¹ Алекперли, Ф.А., Аскерова С.Ф., Симуляция системы управления технологическими процессами и адаптация ее программного обеспечения к промышленным условиям // Вестник компьютерных и информационных технологий. –Москва: –2018, №9 (171),–с.39-48.

"Automation and Control" of the Sumgayit State University, which allows you to implement transfer functions of an arbitrary order with delay.

The paper presents function programs that are implemented in the LAD language and contain 5 independent Network components. In Fig.11. Screen (Screen) is given to visualize the process of local control of the state of the system.

Figure 11 shows the transient processes when the controller setting is changed from 0.22 to 0.27. The time for controlling the degree of catalyst coking at the reactor outlet is 400 seconds, and the transitions from one balanced state to another for the degree of residual coking on the catalyst at the regenerator outlet is 460 seconds, for temperatures in the reactor and regenerator 450 seconds.

THE MAIN RESULTS OF THE DISSERTATION WORK

1. Conducting a review of the literature, it was revealed that the problem of mathematical modeling in order to control the processes of hydrocarbon dehydrogenation in a wide range of changes in phase variables has not yet been worked out.

2. Taking into account the special importance of estimating the degree of catalyst coking in solving the problem of controlling the thermal regime of the technological process and optimizing the yield of the target product, it turns out to be promising to formulate the problem of model estimation of the indicated, physically not measurable parameters.

3. Studies show that the success of solving the set control problem is closely related to the problem of indirect estimation of coke deposition depths based on a dynamic model, the creation of which can be favored by the kinetic approach to describing the thermal processes of exothermic reactions. Based on the theory of chemical kinetics, a model of thermal dynamics was developed, which includes

both the degree of coking of the catalyst after the reaction and regeneration.

4. A special regeneration mode occurs when the system is subjected to emergency heating by supplying additional gas to the regenerator. In this situation, the mathematical model needs structural changes, which consist in a two-phase description of the fluidized catalyst bed in the system. This problem is solved taking into account the mass transfer processes that take place between the dense and rarefied phases of the fluidization bed.

5. The porosity of the catalyst structure makes it necessary to take into account the processes of oxygen mass transfer through internal microscopic channels, as a result of which it is effective to use a fractal description of the catalyst structure in the model being developed.

6. The problem of parametric identification of the hydrocarbon dehydrogenation model has a peculiarity in that parametric identification must be carried out both according to the data of the equilibrium operating modes of the installation, and according to some data of the active experiment of the transition states of the system. In this regard, a mismatch function of a special type is introduced, which contains both the deviation in static states and in the dynamics of transient modes.

7. Due to the importance of visualization of the control process, it is proposed to approximate the system by a third-order expression. The efficiency of this procedure depends on the accuracy of the local stabilization system for one of the coordinates of the dynamical system.

8. A schematic diagram of an indirect measurement system based on a dynamic model of the isobutane dehydrogenation process has been developed, based on the parallelism of movements "object - model" for a given initial condition.

10. Studies have shown that the availability of a mathematical model that satisfies the required dynamic accuracy can play an important role in the creation of high-quality local ATS due to the favorable conditions for their tuning. In operation, these systems are

built using TIA (Totally Integrated Automation) environment modules.

LIST OF PUBLISHED SCIENTIFIC WORKS ON THE TOPIC OF THE DISSERTATION

1. Нагиев, А.Г., Амрахова, Н.А. Моделирование нестационарных тепловых режимов реакторного блока установки кк для пуска и управления в критических ситуациях// Азербайджанский химический журнал. –Баку: -2000, №4. -с.40-45.

2. Нагиев, А.Г., Мамедов, Дж. И., Гулиева, Н.А. Моделирование нестационарных процессов переноса вещества и адсорбции в пористой среде на основе фрактала «Дендрит»// Химия и химическая технология.- Иваново: -2014. т:57, №8. -с.80-84.

3. Гулиева, Н.А. О фрактальном представлении структуры высокопористых твердых катализаторов для математического моделирования адсорбционных процессов// Doktorantların və gənc tədqiqatçıların XIX respublika elmi konfransinin materialları. -Bakı: -2015, - с.169-170

4. Нагиев, Г.А., Гулиева, Н.А. Об аппроксимации решений моделей реакторов вытеснения для описания их нестационарных режимов функционирования// Akademik Toğrul Şaxtaxtınskinin 90 illik yubileyinə həsr olunmuş respublika elmi konfransı. -Bakı: -2015, - с.84.

5. Алиев, А.М., Нагиев, Г.А, Гулиева, Н.А. Об эволюции функций распределения концентрационных и температурных полей в моделях химических реакторов вытеснения и проблема описания траекторий // Сумгаитский государственный университет. Научные Известия. Серия: Естественные и технические науки. –Сумгаит: -2015.т:15, №1, - с.50-54

6. Нагиев, Г.А., Садыгов В.В., Гулиева Н.А. Жесткие системы дифференциальных уравнений и пути совершенствования алгоритмов численного решения // Сумгаитский государственный университет. Научные Известия.

Серия: Естественные и технические науки. –Сумгаит: 2016, т:16, №2, - с.61-65

7. Нагиев, Г.А., Садыхов, В.В., Гулиева, Н.А. Алгоритмизация численного анализа динамичных систем с дифференциально-алгебраическими связями. // интеллектуальные технологии в машиностроении.международная научно-техническая конференция. – Баку: - 2016, -с.48-50. Bakı Dövlət Universiteti

8. Нагиев, Г.А., Садыхов, В.В., Гулиева, Н.А. Дендритовая модель пористого зерна адсорбента как пространственно-геометрический объект со свойством фрактальности//III Respublika elmi konfrans. Riyaziyyatin tətbiqi məsələləri və yeni informasiya texnologiyaları. -Sumqayıt: - 2016, - с.149

9. Гулиева, Н.А. О численном решении модельных уравнений механических систем с вариаторами// Doktorantların və gənc tədqiqatçıların XXI respublika elmi konfransı.-Bakı: -2017, –с. 42

10.Нагиев, Г.А., Гулиева, Н.А. Двухфазная модель структуры кипящего слоя катализатора для моделирования процессов дегидрирования углеводородов// Международная научно-техническая конференция, посвященная дню химика и 40-летию кафедры химико-технологических процессов филиала уфимского государственного нефтяного технического университета г. Салават-Уфа:- 2017, -с.189-190

11.Гулиева, Н.А. Математическое моделирование для управления тепловыми режимами реакционно-регенерационной системы, осуществляющей дегидрирование изобутана// Сумгаитский государственный университет. Научные Известия. Серия: Естественные и технические науки. –Сумгаит:.-2018, т:18, №2, - с.66-70

12.Нагиев, Г.А., Гулиева, Н.А. Моделирование каталитических процессов дегидрирования с учетом меняющейся валентности хрома // Международная научная конференция, информационные системы и технологии: достижения и перспективы. -Сумгаит: -2018,- с.155-157

13.Нагиев, А.Г., Нагиев, Г.А., Гулиева, Н.А. О структуре пространства состояний тепловой модели реакционно-

регенерационных систем с кипящим слоем катализатора и принципах визуализации управления // Теоретические основы химической технологии. –Москва: -2019. -т:53, №1.- с.31-45.

14. Нагиев, Г.А., Гулиева, Н.А. Об одном подходе к снижению размерности динамической системы для визуализации управления на примере процесса дегидрирования углеводородов//Informasiya sistemləri və texnologiyalar nailiyyətlər və perspektivlər. II beynəlxalq elmi konfransi. –Sumqayıt: -2020, с. 40-42

15.Нагиев, Г.А., Гулиева, Н. А. Косвенная оценка переменных состояния реакционно-регенерационных систем на основе компьютерной симуляции// Измерительная техника. –Москва: –2021, № 8.-с.41-49.

16. Гулиева, Н.А. Оперативный контроль степени закоксованности катализатора в реакционно-регенерационных системах по измерениям их температурных координат// прикладные вопросы математики и новые информационные технологии, IV Республиканская научная конференция. -Сумгаит: -2021, - с.237-239

17.Гулиева Н.А. Снижение степени свободы четырехмерной модели системы реактор-регенератор для визуализации управления процессом дегидрирования углеводородов // -Bakı: Azərbaycan Ali Texniki Məktəblərinin Xəbərləri, - 2022, с.17. №6, -s.156-164.

Personal activity of the plaintiff in cases with co-authors:

[1,2] - Parametric identification of the porous structure of the catalyst based on the dendritic fractal and application to the model;

[4] - Estimation of parameters of chemical kinetics of ideal compression model;

[5] - Estimation of hydrodynamic parameters of the model of reciprocating motion in catalyst transport lines;

[6] - Determination of speed coefficients in the kinetic equation of a chemical process

[7] - Programming the problem of choosing the optimal step for the numerical solution of a differential-algebraic coupled system;

[8,10] - Determination of the kinetic coefficients that determine the temperature dependence of the reaction rate coefficients in the dehydrogenation process;

[10] - Estimation of interfacial mass transfer coefficients in the fluidized bed model;

[13] - Parametric identification and computer solution of the dynamics model of reaction-regeneration systems with a fluidized bed;

[14] - Synthesis of a system for automatic control of the reactor temperature in the process of hydrocarbon dehydrogenation;

[15] - Mathematical modeling and calculation of measurement accuracy for indirect measurements;

The defense will be held on the __03 may_____, 2024 at _14:00___ at the meeting of the Dissertation Council ED 2.04 of Supreme Attestation Commission operating under the President of the Republic of Azerbaijan operating at Azerbaijan Technical University.

Address: AZ 1073 Baku, H.Javid Avenue 25

Dissertation is accessible at the Azerbaijan Technical University Library.

Electronic version of the abstract is available on the official website of the Azerbaijan Technical University

Abstract was sent to the required addresses on _02 april__2024

Signed for print: 29.03.2024

Paper format: A5

Volume: 47120

Number of hard copies: 100