Software implementation of the dynamic model of the first stage of the reactor unit for styrene production in the MATLAB/SIMULINK environment

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Abstract. A mathematical description of the physicochemical processes occurring in the first stage of ethylbenzene dehydrogenation in a two-stage adiabatic continuous reactor is developed. A software implementation of the resulting model in Matlab/Simulink environment is presented, that allows to simulate the sequence and dynamics of the flow of internal processes during the equipment operation, taking into account the decrease in activity of the catalytic layer. The algorithm of functioning, structure and model of information flows of the created software, implementing a modular approach to the description of a series-parallel system of thermal, chemical processes and processes on the surface of the catalytic layer are given. The created software allows to simulate the operation of the reactor stage when process parameters change.

1. Introduction and formulation of the task of scientific research

The two-stage reactor unit of the process section of ethylbenzene dehydrogenation in the styrene production is a complex process plant. Its uninterrupted, trouble-free and coordinated operation with other equipment of the process line is provided by a multi-level automated control system (ACS) with a complex structure.

According to the results of the system analysis of the reactor unit as a control object, and also considering its design features and physicochemical regularities of the processes, it is advisable to consider the reactor stages as two separate, sequentially connected process objects with rigid connections, where the output parameters of the first section are input actuation for the second section [1]. From the point of mathematical modeling and automatic control theory, the most complex functional unit of this production system is the first stage of the reaction equipment. The object under consideration consists of mixing zone of vapor of ethylbenzene mixture with superheated water vapor (of mixing chamber) and reaction (catalytic) zone in which chemical reactions with endothermic effects take place.

During the passing of the multicomponent gaseous medium through the reactor stage, a sequential behavior of the heat process in the mixing chamber and the heat and chemical processes in the reaction zone (decomposition of ethyl benzene, deactivation of the catalytic layer, heat absorption along the length of the equipment) occurs. Presented in figure 1 diagram of the processes in the reaction and mixing zones of the reactor shows the sequence of their behavior.
Figure 1. Simplified process diagram of the first stage of the dehydrogenation reactor.

\( R_p \) – water vapor consumption, tons/h.
\( R_{sh} \) – consumption of ethylbenzene mixture, tons/h.
\( R_{sm} \) – consumption of vapor ethylbenzene mixture, tons/h.
\( T_p \) – water vapor temperature at the inlet to the mixing chamber, °C.
\( T_{sh} \) – temperature of the ethylbenzene mixture at the inlet to the mixing chamber, °C.
\( T_{sm} \) – current temperature of the vapor ethylbenzene mixture, °C.
\( a \) – catalyst activity.
\( C_{coke} \) – coke concentration in the catalytic layer, wt.\%.
\( C_{st} \) – styrene concentration, wt.\%.
\( T_{sm,i} \), \( T_{sm,o} \) – the temperature of the reaction mixture at the inlet and at the outlet from the reactor stage, respectively, °C.

This system is a series-parallel (combined). Therefore, based on:
- complexity and continuity of the ongoing heat and chemical processes;
- stiffness of relationships between the values of the process parameters and the quantitative content of the components of the vapor ethylbenzene mixture in the reaction zone;
there is no possibility to predict changes in the values of the main process parameters and determine the state of the control object at arbitrary point in time. This, in turn, does not allow tuning the control system and its adaptation during operation in order to minimize energy and resource costs.

The improvement of the control system of the reactor unit requires its comprehensive study based on the methods of mathematical modeling, as well as numerical methods for optimizing and solving the problems of the process control system. The complexity of the technological processes under consideration requires a significant number of computational experiments, as well as ability to control the course of experiments with the subsequent automated processing of the obtained results.

In modern production conditions, the most effective approach to the improvement of automated control systems aimed at reducing the overall energy intensity of this process is the use of a computer simulation method implemented in the framework of model-based design, which is one of the modern paradigms of control systems development.

The selected concept allows us to investigate the dynamics of object on the basis of the complex mathematical model of its internal processes, without using a real-life reactor or its physical prototype.
At the same time, a virtual simulation of the reactor unit operation as a dynamic system by means of a logical-mathematical description of physical and chemical processes, continuously flowing in its component parts, is not possible without software implementation.

The process of model oriented design of the first stage control system of industrial dehydrogenation reactor can be divided into the following steps:

1. Development of mathematical description.
2. Creation of software (numerical model) imitating the operation of the control object.
3. Verification of the numerical model.
4. Download the program to the hardware complex (computer), ensuring the implementation of calculations in hard real-time mode.
5. Seminatural simulation and research of the reaction equipment operation.

Thus, to build a trusty predictive horizon of the dynamics of the control object, the creation of an automated research system (ASR) for a dehydrogenation reactor is required.

2. Materials, methods and software of research

The investigation of the dynamics and prediction of the object's behavior under various modes of industrial operation is most efficiently carried out using an engineering approach to modeling based on a modular representation of the mathematical description of the process equipment, followed by the implementation of computer models of the processes in the form of software blocks that are components of ASR [2-7].

The analysis of internal processes led to the conclusion that the initial task in the development and implementation of mathematical description for the automated control system of reactor stage is its decomposition into a number of rigidly interrelated elements: a model for the heat exchange process of mixing of charge vapors and water vapor; a model for the heat exchange process inside the reaction zone; a model for the deactivation of catalytic layer; mathematical description of the kinetics of chemical transformations. The mathematical description is the following system of differential equations:

\[
\begin{align*}
\frac{dG_A}{dl} &= a(l) \cdot (k_1(l) \cdot G_B - k_2(l) \cdot G_A \cdot G_B), \\
\frac{dG_B}{dl} &= a(l) \cdot (k_2(l) \cdot G_A \cdot G_B - k_3(l) \cdot G_B - k_4(l) \cdot G_B \cdot G_C), \\
\frac{dG_C}{dl} &= a(l) \cdot (k_3(l) \cdot G_B - k_2(l) \cdot G_A \cdot G_B - k_4(l) \cdot G_B \cdot G_C), \\
\frac{dG_D}{dl} &= a(l) \cdot k_3(l) \cdot G_B, \\
\frac{dG_E}{dl} &= a(l) \cdot k_3(l) \cdot G_B, \\
\frac{dG_F}{dl} &= a(l) \cdot k_4(l) \cdot G_B \cdot G_C, \\
\frac{dG_G}{dl} &= a(l) \cdot k_4(l) \cdot G_B \cdot G_C, \\
\frac{dT}{dl} &= \frac{\Delta H \cdot G_A(l) \cdot S \cdot l \cdot M_A}{C_{th}(l) \cdot \rho_0 + c_p(l) \cdot \rho_0} \\
&\quad - \frac{Ea}{k_{koc_{max}} \cdot k_{koc}(T(l))} \\
a(l) &= e^{-\frac{Ea}{k_{koc_{max}} \cdot k_{koc}(T(l))}} \\
k_i(l) &= k_0 \cdot e^{-\frac{RT(l)}{Ea}}, i = 1..4 \\
G_A \bigg|_{l=0} &= G_C \bigg|_{l=0} = G_E \bigg|_{l=0} = G_F \bigg|_{l=0} = 0 \\
G_B \bigg|_{l=0} &= 52.266, G_D \bigg|_{l=0} = 0.071 \\
G_F \bigg|_{l=0} &= 0.060
\end{align*}
\]
where
\( v \) is the linear flow rate of the ethylbenzene mixture (charge), m/s;
\( G_A, G_B, G_C, G_D, G_E, G_F, G_g \) – concentrations of styrene, ethylbenzene, hydrogen, benzene, ethylene, toluene, and methane, respectively, mol/l;
\( k_1 \) is the rate constant for the formation of styrene and hydrogen (direct stage of the dehydrogenation reaction), s\(^{-1}\);
\( k_3 \) is the rate constant for the formation of benzene and ethylene, s\(^{-1}\);
\( k_2 \) is the rate constant of the reverse dehydrogenation reaction, l/(mol \cdot s);
\( k_4 \) is the rate constant for the formation of toluene and methane, l/(mol \cdot s);
\( G_A(l) \) – the current value of the concentration of released styrene, mol/l;
\( C^{sh}(l) \) – the current value of the heat capacity of the charge, J/(kg \cdot K);
\( c^p(l) \) – current value of heat capacity of water vapor, J/(kg \cdot K),
\( m_0^{sh} \) – consumption of the charge, kg/s;
\( T_0^{sh} \) – charge temperature at the inlet to the mixing chamber, K;
\( c_0^p \) – specific heat of water vapor at the inlet to the reaction zone, J/(kg \cdot K);
\( m_0^p \) – consumption of water vapor, kg/s;
\( \Delta H = 1130436 \) – the amount of energy expended on the formation of one kilogram of styrene, J/kg;
\( S \) is the cross-sectional area of the reactor, m\(^2\);
\( k_0 \) is the preexponential factor;
\( E_a \) is the activation energy of the dehydrogenation reaction, J/mol;
\( R \) is the universal gas constant;
\( T \) is the temperature in the reactor, K;
\( l \) is the length of the reactor stage, m;
\( M_A \) – molar mass of styrene, kg/mol;
\( a(l) \) is the catalyst activity;
\( K_{kokc_{max}} \) – the maximum concentration of coke on the catalytic layer, wt.%;
\( K_{kokc}(l) \) – the current value of the concentration of coke, wt.%.

The effectiveness of the proposed approach cannot be provided by a program developed without the use of specialized integrated environments, application packages and computer-aided design systems that allow to accelerate and automate the software synthesis stages for scientific and industrial research.

To implement the virtual work of the reactor stage, it is advisable to use CASE-programming technology that allows to combine the system analysis tools, design and perform technical calculations in the development environment, as well as effectively solve the problems of logical, algorithmic and mathematical connection of software modules. Therefore, the Matlab system, where the interactive graphical environment Simulink was used as a software development tool, was chosen.

As a result of creating and debugging software blocks, a computer software is implemented as a composition of mathematical modules describing the change in process parameters and concentration profile of chemical reaction products along the length of the reactor stage [8, 9].

The final and most difficult stage in creating of software tool for research is the compatibility of mathematical elements at the macro level and modules for the fundamental description of facts and reactions at the micro level. Therefore, simulation modeling of operation of the industrial plant of styrene production requires compliance of input, output parameters and variable modules of the mathematical description to ensure the closedness of the heat exchange equations, chemical kinetics and processes of coke formation on the catalyst.

In figure 2 presents the screen interface of the starting form of the dehydrogenation process calculation program. The software is developed on the basis of the built-in mechanism for creating vir-
tual subsystems of the Simulink environment planted in the “Subsystem” functional block. Structurally, software is a hybrid of executable macro and micromodules. The instrumental capabilities of the development environment and the flexibility of tuning these blocks provide for the calculation and synchronization of data exchange between the models of the processes taking place in accordance with the developed algorithm for calculating the model and the used numerical method for solving equations describing the kinetics of chemical transformations.

Figure 2. The starting form of the program for calculating of mixing chamber and reaction zone of the reactor in Simulink.

The starting form includes two macroblocks (subsystems): “Subprogram of calculating the process of mixing vapor of raw materials and water vapor” and “Subprogram of calculating physical and chemical processes in the reaction zone of the reactor stage”. It allows to simulate of processes in two structurally separated parts of the reaction stage: the mixing chamber and the catalytic decomposition zone of the ethylbenzene mixture. Software architectures of the main software modules are shown in figure 3 and figure 4 respectively.

In the process of the macromodule operation “The module for calculating the heat exchange process in the mixing chamber”, the screen form of which is shown in figure 3, with using the “Subsystem” elements, being micromodules in this subprogram, a sequential calculation is performed for:
- values of heat capacities of the components of ethylbenzene mixture and water vapor at the inlet to the mixing chamber (micromodule 1 and micromodule 2);
- temperature of the vapor-ethylbenzene mixture at the outlet of the mixing chamber (micromodule 3);
- values of heat capacities of the components of ethylbenzene mixture and steam at the outlet from mixing zone (micromodule 4 and micromodule 5);
- calculation of the linear flow rate of the vapor-ethylbenzene mixture.

Figure 3. Subprogram for calculating the process of mixing ethylbenzene vapor and water vapor.

Figure 4. Subprogram for calculation of physical and chemical processes in the reaction zone of the reactor stage.
The software architecture of the unit for performing calculations of the charge dehydrogenation stage, shown in figure 4, is also a set of micromodules, each of which calculates the dynamics of the flow of the elementary process inside the catalytic section of the reactor.

As a result of synchronization of data exchange between the corresponding inputs and outputs of the micromodules, the process of modeling the control object is performed according to the following algorithm:

1. Calculation of the rate constants of chemical reactions (micromodule 1).
2. Solving the system of differential equations describing the dynamics of changes in the concentrations of components of the contact gas along the length of the reaction stage (micromodule 2).
3. Determination of the rate of fall of the values of the total specific heat and heat capacities of the components of the vapor ethylbenzene mixture as a result of changes in its composition and temperature (micromodule 3 and micromodule 4).
4. Simulation of heat exchange processes in the reaction zone: determination of the value of the change in temperature of the reaction mixture along the length of the reactor stage, thermal effect evaluation of the chemical dehydrogenation reaction (micromodule 5).
5. Calculation of the amount of coke deposited on the catalyst and determination of the degree of its deactivation (micromodule 6).

The micromodules indicated at the 1st, 3rd and 4th stages of the algorithm are implemented using the “Subsystem” block. The micromodule used at the 2nd stage is created on the basis of block - editor of differential equations. The kinetic model is calculated using the built-in algorithm for implementing the numerical method of solving 4th order Runge-Kutta systems of ordinary differential equations. The information flow model of the software is shown in figure 5.

![Figure 5. DFD-model of information flow of software.](image)

where, data and results of mathematical modules calculations, transmitted in the information flow of software, represented by one and multi-element tuples:

- `<xa, xb, xc, xd, xe, xf, xg, xp>` - mass fraction of styrene, ethylbenzene, hydrogen, benzene, ethylene, toluene, methane and water vapor at the entrance to the mixing chamber of the reactor, mass/share;
- `<k1, k2, k3, k4>` - current values of the chemical reactions rate constants, l/(mol×s);
<Ma, Mb, Mc, Md, Me, Mf, Mg, Mp> - mass of styrene, ethylbenzene, hydrogen, benzene, ethylene, toluene, methane and water vapor at the entrance to the mixing chamber of the reactor, t/h;

<Ga, Gb, Gc, Gd, Ge, Gf, Gg, Gp> - concentration of styrene, ethylbenzene, hydrogen, benzene, ethylene, toluene, methane and water vapor at the entrance to the mixing chamber of the reactor, mol/l;

<k1, k2, k3, k4> - initial values of the chemical reactions rate constants, l/(mol×s);

<P> - pressure in the reaction zone, kg/cm²;

<dL> - step size along the length of the reaction zone, m;

<L> - the length of the reactor stage, m;

<Rsh> - mass flow rate of ethylbenzene, t/h;

<Rp> - mass flow rate of water vapor, t/h;

<Tsh> is ethylbenzene temperature, °C;

<Tp> is the temperature of water vapor, °C;

<Csm> - specific heat capacity of the vapor-ethylbenzene mixture, J/(kg×K);

<Rsm> is the mass flow rate of the vapor-ethylbenzene mixture, t/h;

<Tsm> is the temperature of the vapor-ethylbenzene mixture, °C;

<Qsm> - a vapor ethylbenzene mixture amount of heat, J;

<U> - linear flow rate of a vapor ethyl benzene mixture, m/s;

<a> - catalytic layer activity, %.

3. Software performance

The Matlab application package is equipped with a wide range of software and graphic tools that allow to effectively present and analyze data of changes in the parameters of the reaction mixture obtained as a result of the operation of simulation program for the dehydrogenation process. The results of the investigation of the dynamics of the control object while varying the values of the reactor load by raw materials (charge consumption) are presented in figure 6 - 8 in the form of three-dimensional graphic functions showing the change in the process of reactor operation for such parameters as: the heat capacity of the components of the vapor-ethylbenzene mixture; the temperature of the reaction mixture; the styrene concentration.

Analysis of the results of the developed software application has showed that the reaction mixture during the passing through the catalytic layer absorbs the amount of heat causing a decrease in temperature at 40 ÷ 50 °C and a decrease in the total specific heat and heat capacities of the components of the contact gas, which is confirmed by the nature of the change of these values depending on the temperature mode of reactor operation [11].

![Figure 6. Graph of changes in styrene concentration along the length of the reactor stage at various values of ethylbenzene charge consumption.](image-url)
Figure 7. Graphs of changes in the heat capacities of the main components of the vapor ethylbenzene mixture: a) styrene, b) benzene; c) toluene; d) ethylene; along the length of the reaction zone.

Figure 8. Dynamics of the contact gas temperature drop along the length of the first stage of the reactor unit.
4. Conclusion
The developed software, consisting of a set of subprograms executed in the form of functional flowcharts, is a convenient and versatile tool that simulates the dynamics of the first stage of ethylbenzene dehydrogenation while varying the values of the process parameters. At the same time, Matlab environment provides the ability to integrate functional blocks of Simulink libraries with executable (by the command) files that perform procedures created by the classical way of programming in the same built-in high level language. It provides ample opportunities for: further improvement and interactive calculation of the mathematical description of the process, automation of computational experiments, fast and effective conversion of the simulation model to the control object model operating in hard real-time mode, taking into account internal and external disturbances, compiling the program code with the aim of use in a programmable logic controller, which is part of the automated program control system of reactor unit.

Thus, in the Matlab/Simulink environment, the simulation model of the first stage of the ethylbenzene dehydrogenation reactor was developed, that implements the virtual simulation of the process object operation. The computational experiments have showed that the developed mathematical description allows qualitatively describing the processes occurring in the object under investigate, and also confirmed the correctness of the operation of the created Simulink program, which is a tool for scientific research of the reaction apparatus as a dynamic system and the basis for conducting the seminatural simulation of its operation.

References
[1] Popov A, Bitukov V, Tikhomirov S and Neizvestny O 2018 J. Vestnik VSUET 80 77-85
[2] Shelepova E, Vedyagin A, Mishakov I, Noskov A 2014 Catalysis for Sustainable Energy 2 1-9
[3] Abdelhamid Ajbar, Emaddine Ali 1998 J. King Saud Univ. 10 141-62
[4] Jackson G 2012 Chemical and Process Engineering Research 3 14-28
[5] Bashirov N, Ali Riza Kul 2012 International Journal of Applied Science and Technology 10 133-41
[6] Sheppard C, Maler E, Caram H 1986 Eng. Chem. Process Des. Dev. 25 207-10
[7] Hossain M, Atanda L, Al-Yassir N, Al-Khattaf S 2012 Chemical Engineering Journal 207-208 308-21
[8] Zhatova I, Popov A, Alekseev M 2014 Nauchny vestnik VSUACE 4 80-83
[9] Bitukov V, Popov A, Tikhomirov S and Neizvestny 2017 Vestnik VSUET 79 73-80
[10] Zhorov Y 1985 Thermodynamics of chemical processes Moscow Chemistry 220-40