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Computer Modeling of Chemical Process Systems with Distributed Parameters by Means of Component Circuit Method with Non-Uniform Vector Coupling

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Abstract

The paper considers a method for modeling chemical process systems (CPSs) of gas industry enterprises in the form of a component circuit method with the application of non-uniform vector connections. It is used as a foundation for a multilevel computer modeling environment that allows automating solutions of problems in CPS research and functional design.

Keywords: *Chemical process system; Non-uniform vector connection; Component circuit method; Heat exchanger; MARS modeling environment.*

1. Introduction

Gas industry facilities commonly include complex technical controlled system, having the form of a complex of process equipment and consisting of a controlled chemical process system (CPS) and a control device (CD), which are linked by the executive and measuring devices. A CPS may be decomposed into mutually linked elements that have controlled energy and matter streams of various nature between them. The functioning scenario of the CD includes several parallel algorithms with common memory space. Each of them provides obtaining values of observed characteristics from measuring devices (transmitters), their mathematical (numeric) processing, and data visualization, which is used as a base for operator's development of control actions with the aim of maintaining a necessary mode of operation under the influence of various perturbations.

It is rational to use computerized CPS control systems for automatic solution of problems in research, design, and control of CPS, as well as for implementing various teaching modules. The existence of energy and material links, both direct and reverse, and coefficients in equations of the mathematical model of a CPS element or apparatus being dependent on hydraulic and thermodynamic characteristics, concentrations, and flow parameters complicate the implementation of CPS computer models and computational experiments.

Implementation of software and algorithmic apparatus for computer modeling of chemical process systems on the basis of numerical experiment provides possibilities to automate the following tasks in research and functional design of CPSs:

– structure formation, selection of CPS elements, and determining the values of their parameters that allow for given modes of operation;
– the selection of executive devices that have direct energy influence onto CPS, proportional to information signals from CD and intended for maintaining a required state or transition to a new state;
– development and debugging of operational scenarios of Scada-system that provide computerized, including AI-informed control of CPS with CD included into the control loop for automatic solution of tasks in determining, setting, and maintaining required modes of operation;

– development of computer education programs and network-based computer training packages for process control operators involved in the control of processes within a CPS.

A universal method of computer modeling and automation of simulation experiments of multiphysical nature is a component circuit method (CCM) [1-2]. Originally proposed by VM Dmitriev and EA Arais, this method is currently adapted to modeling technical devices and systems [3].

This paper demonstrates the development of the CCM for modeling chemical process systems with distributed parameters and variables along with the whole chemical processing technology. It consists in a theoretical justification of the non-uniform vector relationship apparatus with subsequent implementation of relevant software and algorithmic framework for creating numerical models of CPSs and their subsequent analysis with a universal calculation core [4] of MARS modeling environment [5], which is implemented on the basis of the CCM.

2. Generalized structural and functional diagram of a CPS

Chemical process systems [6] of gas industry enterprises involve physical and chemical transformations of multicomponent matter flows under the management of process operators interacting with APCS and SCADA systems. Hydraulic and thermodynamic characteristics of the flows are subject to change, as well as their composition. The changes include phase transitions of some components (substances) [7-8], as well as various chemical reactions resulting in obtaining new substances, hereinafter called *flow components*. CPS is a set of elements and apparatuses where several multicomponent matters flow interact. Each separate apparatus is a physical and chemical system (PCS), where a certain process of physical or chemical transformation takes place, involving multicomponent mixtures of substances in the liquid or gaseous phase. In order to obtain the desired result, these flows of certain temperature *T* and flow rate *G* shall be supplied to a relevant apparatus at a pressure of *P*. A generalized CPS, implemented in the form of a single apparatus and having executive devices and measuring instruments for pressure and temperature may include the following components (Figure 1):

– *IS*1, *IS*2 are controlled sources of multicomponent substance mixtures, where the substance flowrate *G* is regulated;
– RC1, RC2, RC3, RC4 are pipes that exert hydraulic and thermodynamic resistance on the multicomponent flow passing through them;
– N1, N2 are controlled pumps that increase the pressure of a flow within the PCS by a certain value of Δ*P*;
– T1, T2 are controlled heaters that increase the temperature of the multicomponent mixture supplied to the CPS by a value of Δ*T*.

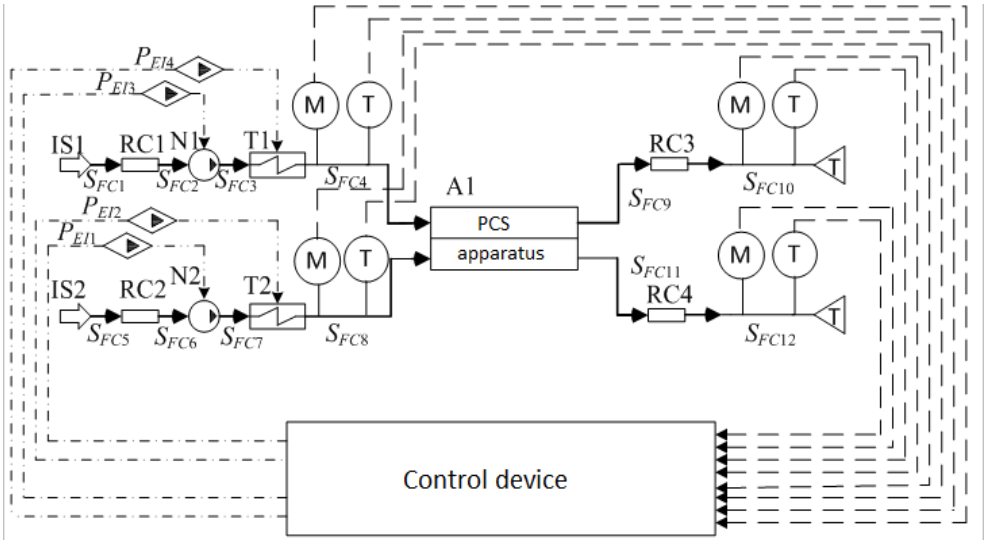

Fig. 1. Functional diagram of a generalized chemical process system

A feature of such apparatuses measures the rate of the process and characteristics of the substances along with the PCS apparatus. Description of such phenomena uses partial derivative equations along the length of the apparatus in question.

Observation over the processes taking place in the CPS is performed with gages M and thermometers T, which measure the pressure and temperature of the mixture in the points where their sensing elements are installed. Measuring results are transformed into information signals to be transmitted to CD by energy-information transducers P_{EI1}, …, P_{EI6} [9]. Control over processes in each CPS apparatus is performed with pumps N1 and N2, as well as heaters (coolers) T1 and T2.

Relations between the CPS components S_{FC1}, S_{FC2}, …, S_{FC12}, being physico-chemical ones, describe the energy characteristics and concentrations of substances in the multicomponent flows modeled by the relations. Each relation may be represented in the form

$$S_{FCi} = \{S_{Gi} \cup S_{Ti} \cup S_{Ci}\} \rightarrow \{\{P_i, G_i\} \cup \{T_i, Q_i\} \cup \{\mathbf{C_i}\}\}, \quad (1)$$

where $S_{Gi} \rightarrow \{P_i, G_i\}$ is a hydraulic relation where P_i is the pressure and G_i is the volume flow of the substance; $S_{Ti} \rightarrow \{T_i, Q_i\}$ is a thermodynamic relation consisting of temperature T_i and thermal flow Q_i; $S_{Ci} \rightarrow \{C_i\}$ is a uniform vector relation containing concentrations of all the components (substances) of a given flow.

The problems of constructing and studying mathematical and computer models of CPSs are concerned in the works of VV Kafarov, VP Meshalkin, IN Dorokhov [6,10-11]. The issues of applying modeling software complexes to CPS modeling as exemplified by HYSYS in both R&D and teaching were considered in the works of TN Gartman [12]. The problems in the development of computer models of CPS for process control were analyzed by scientists from the Tomsk Polytechnic University [13-17].

Currently, control of processes within CPSs employs automated control systems, functional design, and smart control processes [18], where they are current developments. The scale of the objects and complexity of the processes, together with the requirements to set and maintain corresponding operational modes of the process equipment, do not allow for training and further training of gas industry personnel using real operating equipment. In order to solve these tasks, CPS computer models are required, implemented within the framework of a universal computer modeling method that allows bringing components together in a unified model, including components with both continuous and discrete-event behavior.

In order to automate the research tasks and CPSs, this work employs the component circuit method [1]. Being a universal method of computer modeling, it allows:

– forming and automating the analysis of CPS computer models that permit decomposition into elements where each element may be represented as a *component* – a substitute model that describes the transformation of energy and matter flows in the element with a system of algebraic differential equations;
– composing simulation models for automated experiment scenarios aimed as solving the tasks in CPS research and functional design;
– visualizing results from the analysis of CPS models in static and dynamic modes using display facilities, virtual tools, and instruments [19].

In order to implement CPS computer models, a generalized component of the chemical process system was formed in the form of a component circuit with non-uniform vector couplings.

3. Principal concepts of the component circuit method

The basic concepts of the CCM are component and component circuits.

The component is a formalized image of an element, functional block, or apparatus of a CPS in the facility or system being modeled. It has its own mathematical model. It is formed in the local coordinate base of the component as a system of equations compiled with respect to its primary parameters and variables of its relations in the physical coordinate basis.

Component circuit, which is a basic model of the studied object of a system in the CCM, in general case is an unspecified set of components, whose relations, known as *branches*, are connected in common points, so-called circuit *nodes*

$C=(K, B, N)$ (2)

where K is a set of components; B is as set of nodes; N is a set of branches.

Each component in the set K has a set of links; each of them is, in a general case, a non-uniform vector coupling.

3.1. Structure of a non-uniform vector coupling

For the purpose of modeling the transformation of physically non-uniform energy streams and multi-component matter flows in the CPS, component circuits with non-uniform vector coupling (NVC) are employed within the framework of the CN method.

Each non-uniform vector coupling $\mathbf{S_{vk}}$, structure and content of which is shown in Figure 2 is a set of a number of interacting energy and information links

$\mathbf{S_{vk}}=[S_{E\_1k}, S_{E\_2k}, \ldots, S_{E\_Cek}, S_{I\_1k}, S_{I\_2k}, \ldots, S_{I\_Cik}]$, (3)

vector branch $\mathbf{b_k}$ of which is incident to its vector node $\mathbf{n_k}$ and is of the form

$\mathbf{S_{vk}}=(\mathbf{b_k}\ \eta\ \mathbf{n_k})$, (4)

where $\mathbf{b_k}=[b_{k1}\ \ b_{k2}\ \ \ldots\ \ b_{k\mathrm{Ce}}]$ is a vector branch, which is a vector of size Ce of the branch numbers of scalar energy links within the NVC $\mathbf{S_{vk}}$; η is a ratio of incidence of the branch $\mathbf{b_k}$ to a node $\mathbf{n_k}$; $\mathbf{n_k}=[\ n_{k1}\ \ n_{k2}\ \ \ldots\ \ n_{k\mathrm{Ce}}\ \ n_{k\mathrm{Ce}+1}\ \ n_{kCe+2}\ \ \ldots\ \ n_{k\mathrm{Ce}+\mathrm{Ci}}]$ is a vector node of a size $Ce+Ci$, appearing as a vector of node numbers of energy and information links within the vector coupling $\mathbf{S_{vk}}$; Ce is a quantity of energy links; Ci is a quantity of information links in the non-uniform vector coupling $\mathbf{S_{vk}}$.

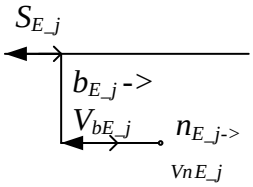

Fig.2. The structure of an energy link

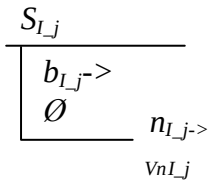

Fig. 3. The structure of the information link

To each energy link S_{E_j} (Figure 2), there is a corresponding pair of topological coordinates, node n_{E_j} and branch b_{E_j} with variables V_{nE_j} and V_{bE_j}, where V_{nE_j} is a potential variable, and V_{bE_j} is a flow variable, hereinafter they are called component link variables

$S_{E\_j} = (b_{E\_j}\ \eta\ n_{E\_jk}) \rightarrow \{V_{nE\_jk}, V_{bE\_jk}\}$; (5)

Each information link S_{I_jk} (Figure 3) is associated with a pair of topological coordinates – a node n_{I_j} and a branch b_{I_j} – with a single potential variable V_{nI_j}

$S_{I\_j} = (b_{I\_j}\ \eta\ n_{I\_jk}) \rightarrow \{V_{nI\_jk}\}$; (6)

Components with non-uniform vector couplings (4) are proposed as a basis for a structure of a generalized component of CPS to be used in modeling the principal elements and apparatuses of chemical technology used in oil and gas processing.

4. Generalized component of a chemical processing system

Process facilities of the oil and gas industry pertain to the class of chemical process systems (Figure 1). Matter flows that circulate between their elements and apparatuses are multicomponent mixtures of substances that have various types of energy. A certain type of energy in each node will be described with a pair of dual variables, where the product of their current values in any moment characterizes the power of the energy, and the energy is going to be described with an energy link in the form of (5).

Matter flow formed by a single substance is going to be considered a single-component flow, while that including several substances will be called a multicomponent flow. A specific substance in the flow is called a component and is characterized by its concentration that defines the substance's mass, volume, or molar ratio in the flow. It will be described with an information link in the form (6).

In order to describe chemical process systems with the multicomponent matter flows, the links are provided with a generalized component of CPS (Figure 4).

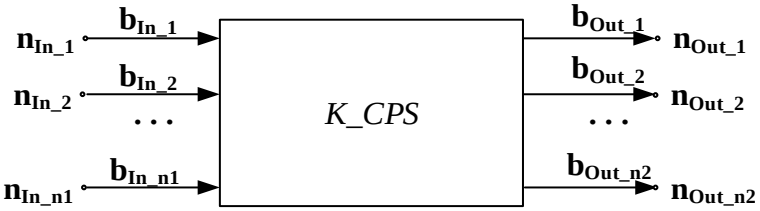

Fig. 4. Generalized component of a chemical processing system

Its inputs $\mathbf{S_{In\_1}}=(\mathbf{b_{In\_1}}\ \eta\ \mathbf{n_{In\_1}})$, $\mathbf{S_{In\_2}}=(\mathbf{b_{In\_2}}\ \eta\ \mathbf{n_{In\_2}})$, …, $\mathbf{S_{In\_n1}}=(\mathbf{b_{In\_n1}}\ \eta\ \mathbf{n_{In\_n1}})$ and outputs $\mathbf{S_{Out\_1}}=(\mathbf{b_{Out\_1}}\ \eta\ \mathbf{n_{Out\_1}})$, $\mathbf{S_{Out\_2}}=(\mathbf{b_{Out\_2}}\ \eta\ \mathbf{n_{Out\_2}})$, …, $\mathbf{S_{Out\_n2}}=(\mathbf{b_{Out\_n2}}\ \eta\ \mathbf{n_{Out\_n2}})$, being of physical-chemical nature (1) are implemented on the basis of a non-uniform vector coupling (3), with $Ce=2$ и $Ci=Cc$, where Cc is the number of substances circulating through all the links of the CPS being modeled.

Each of the links is a set of two energy links and several information links

$$\mathbf{S_j} = \{S_j^G, S_j^T, S_j^{C1}, S_j^{C2}, \ldots, S_j^{Ccf}\}, \quad (7)$$

where $S_j^G=(b_j^G\ \eta\ n_j^G)\rightarrow\{V_{nj}^G=P_j,\ V_{bj}^G=G_j\}$ is the energy link that characterizes the hydraulic energy of the multicomponent matter flow; $S_j^T=(b_j^T\ \eta\ n_j^T)\rightarrow\{V_{nj}^T=T_j,\ V_{bj}^T=Q_j\}$ is the energy link that characterizes its thermodynamic energy; $S_j^{C1}=(b_j^{C1}\ \eta\ n_j^{C1})\rightarrow\{V_{nj}^{C1}=C_1\}$, $S_j^{C2}=(b_j^{C2}\ \eta\ n_j^{C2})\rightarrow\{V_{nj}^{C2}=C_2\}$, …, $S_j^{Ccf}=(b_j^{Ccf}\ \eta\ n_j^{Ccf})\rightarrow\{V_{nj}^{Ccf}=C_{cf}\}$ is the set of information links, each of which characterizes concentration of a specific substance in the flow in question.

As there are processes in the CPS apparatuses that are distributed along the length of the apparatus, in addition to traditional linear, non-linear, and ordinary differential equations, equations in partial derivatives along the apparatus's length have been introduced:

– linear equations with partial derivatives along the length of the apparatus l:

$$\sum_{i=1}^{N} K_i \cdot \frac{dV_i^{K\_CPS}}{dl} = \sum_{i=1}^{N} a_i \cdot V_i^{K\_CPS} + b\,, \quad (8),$$

where K_i, a_i, b are constant factors;

– non-linear equations with linear component partial derivatives

$$\sum_{i=1}^{N} K_i \cdot \frac{dV_i^{K\_CPS}}{dl} = f\left(\mathbf{V^{K\_CPS}}\right) \quad (9),$$

where K_i are constant factors, $\mathbf{V^{K\_CPS}}$ is a variable link vector of the CPS component in question, f is a non-linear function;

– regular differential equations with partial derivatives along the length of the apparatus

$$\sum_{i=1}^{N} M_i \cdot \frac{dV_i^{K\_CPS}}{dt} = \sum_{i=1}^{N} K_i \cdot \frac{dV_i^{K\_CPS}}{dl} + f\left(\mathbf{V^{K\_CPS}}\right) \quad (10),$$

where M_i, K_i are constant factors, f is a non-linear function.

These equations allow using the component circuit method to model the processes inside the apparatuses, study the distribution of hydraulic and thermodynamic characteristics, as well as the concentration of substances along the length of the CPS apparatuses. Let us consider the method used for the formation of computer models of CPS components with distributed parameters and variables through an example of a heat exchanger.

5. Computer model of a heat exchanger in partial derivatives along the length of the apparatus

The heat exchanger is a CPS apparatus where heat energy is exchanged between two transfer mediums; multicomponent matter flows in the gaseous or liquid phase at different

temperatures. There, we may see the transfer of heat from a medium of a higher temperature, hereinafter called hot medium, to a medium of a lower temperature through a wall that separates the mediums. It is assumed that all the thermal energy passes from the hot medium to the cold medium through the wall without any losses. Taking into account that the heat exchange happens through the whole area of medium contact that has a rectangular form, temperature measurements of the hot and cold mediums will be described with a system of differential equations in partial derivatives

$$\begin{aligned}\frac{\partial T^H}{\partial l} &= \frac{K\cdot d}{G^H\cdot CP^H\left(T^H(l)\right)\cdot \rho^H}\cdot\left(T^H(l)-T^C(l)\right)\\ \frac{\partial T^C}{\partial l} &= -\frac{K\cdot d}{G^C\cdot CP^C\left(T^C(l)\right)\cdot \rho^C}\cdot\left(T^H(l)-T^C(l)\right)\end{aligned} \tag{11}$$

where K is a heat transfer ratio; d is the width of the area in the dividing wall; l is its length; G^H, G^C are molar flows of the hot and cold mediums respectively; ρ^H, ρ^C are their densities calculated with the formula

$$\rho = \sum_{i=1}^{N_C}\rho_i\cdot C_i\,, \tag{12}$$

where ρ_i is the density of the i-th component of the flow; C_i is the concentration of the i-th component of the flow; CP^H, CP^C are specific molar heat capacity of the heat transfer mediums, calculated with the formula

$$CP(T) = \sum_{i=1}^{N_C}CP_i(T)\cdot C_i\,, \tag{13}$$

where $CP_i(T)$ is the specific heat capacity of the substances in the relevant heat transfer medium; C_i is their concentrations.

Specific heat capacity values of the substances that depend on temperature are determined with the formula :

$$CP_i(T) = CP\_A_i + CP\_B_i\cdot T + CP\_C_i\cdot T^2 + CP\_D_i\cdot T^3 \tag{14}$$

where $CP\_A_i, CP\_B_i, CP\_C_i, CP_{D_i}$ are constants in the ideal gas density equation where CP is expressed in cal/(mol*K). These constants are calculated for each substance in the flow.

Changes in the heat flow of the hot and cold heat transfer mediums respectively along the whole length of the separating wall of the heat exchanger are described with the equations.

$$\begin{aligned}Q^H(0)-Q^H(L) &= \rho^H\cdot G^H\cdot\left(CP^H\left(T^H(L)\right)\cdot T^H(L)-CP^H\left(T^H(0)\right)\cdot T^H(0)\right)\\ Q^C(0)-Q^C(L) &= \rho^C\cdot G^C\cdot\left(CP^C\left(T^C(L)\right)\cdot T^C(L)-CP^C\left(T^C(0)\right)\cdot T^C(0)\right)\end{aligned} \tag{15}$$

The Heat Exchanger component implemented on the basis of equations (11)–(15) is shown in Figure 5.

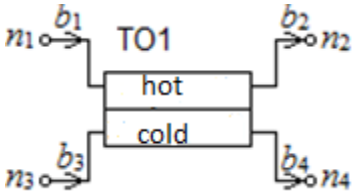

Figure 5. Heat Exchanger Component

It has the following links:

$S_1 = \left(b_1 \eta^- n_1\right) \rightarrow \left\{\left\{P^H(0), G^H(0)\right\}, \left\{T^H(0), Q^H(0)\right\}, C^H(0)\right\}$ is a link (1) through which the hot heat exchange medium is supplied to the heat exchanger;

$S_2 = \left(b_2 \eta^- n_2\right) \rightarrow \left\{\left\{P_2^H(L), G_2^H(L)\right\}, \left\{T^H(L), Q^H(L)\right\}, \left\{C_2^H(L)\right\}\right\}$ is a link (2) through which the hot heat exchange medium leaves the apparatus;

$S_3 = \left(b_3 \eta^- n_3\right) \rightarrow \left\{\left\{P_1^C(0), G_1^C(0)\right\}, \left\{T^C(0), Q^C(0)\right\}, \left\{C_1^C(0)\right\}\right\}$ is a link (3) through which the cold heat exchange medium is supplied to the heat exchanger;

$S_4 = \left(b_4 \eta^- n_4\right) \rightarrow \left\{\left\{P_2^C(L), G_2^C(L)\right\}, \left\{T^C(L), Q^C(L)\right\}, \left\{C_2^C(L)\right\}\right\}$ is a link (4) through which the cold heat exchange medium leaves the heat exchanger.

As the computing core of the MARS modeling environment [4] accepts linear, non-linear, and ordinary differential equations as inputs, differential variables were linearized in partial derivatives (11) according to the implicit Euler method before forming a program code of the heat exchanger model. To that end, the whole length of the heat exchanger *L* is divided into several elementary cells with a constant increment of Δ*l*. For each cell from the equation (11), linearized equations are formed with respect to temperature values at the start *T*(*l*) and at the end of the cell *T*(*l*+Δ*l*).

$$\begin{aligned} G^H(0) \cdot CT\left(T^H(l+\Delta l)\right) \cdot T^H(l+\Delta l) - (1 - K \cdot d \cdot \Delta l) \cdot T^H(l) - K \cdot d \cdot \Delta l \cdot T^C(l) = 0 \\ G^C(0) \cdot CT\left(T^C(l+\Delta l)\right) \cdot T^C(l+\Delta l) - (1 - K \cdot d \cdot \Delta l) \cdot T^C(l) + K \cdot d \cdot \Delta l \cdot T^H(l) = 0 \end{aligned} \quad (16)$$

Formation of equations (16) happens automatically until the value of *l*+ Δ*l* becomes equal or higher than *L*. Other variables at the ends of the cells are determined with the formulas

$$\begin{aligned} Q^H(0) - Q^H(L) - \rho^H \cdot G^H(0) \cdot \left(CP^H\left(T^H(L)\right) \cdot T^H(L) - CP^H\left(T^H(0)\right) \cdot T^H(0)\right) = 0 \\ Q^C(0) - Q^C(L) - \rho^C \cdot G^C(0) \cdot \left(CP^C\left(T^C(L)\right) \cdot T^C(L) - CP^C\left(T^C(0)\right) \cdot T^C(0)\right) = 0 \\ P^H(0) - P^H(L) = 0 \\ G^H(0) - G^H(L) = 0 \\ C_i^H(0) - C_i^H(L) = 0 \\ P^C(0) - P^C(L) = 0 \\ G^C(0) - G^C(L) = 0 \\ C_i^C(0) - C_i^C(L) = 0 \end{aligned} \quad (17)$$

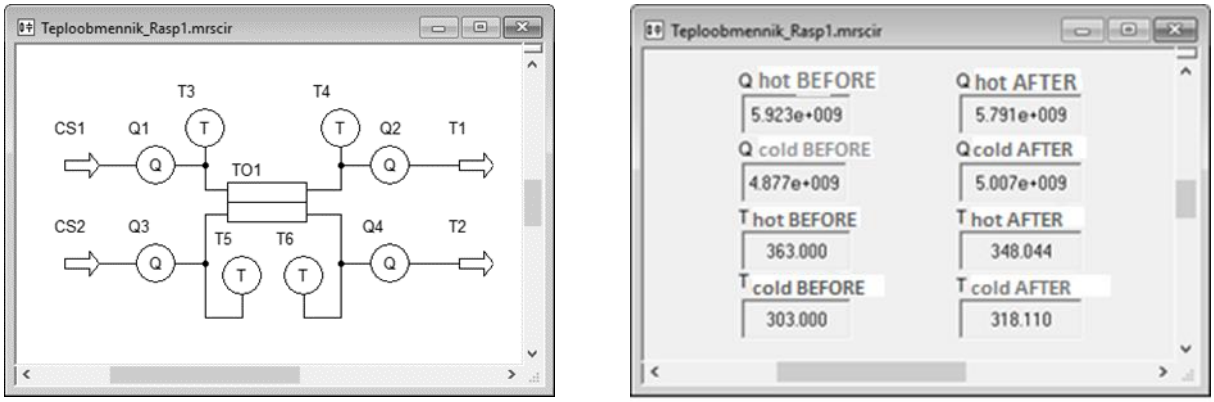

Figure 6. Modeling a heat exchanger
a) computer model of the heat exchanger

b) modeling results

Figure 6 shows a computer model of a heat exchanger where source SC1 supplies hot heat-exchange medium at a pressure of 100,000 kPa, the volume flow rate of 2000 m^3/h, and a temperature of 363 K, while source SC2 supplies cold heat-exchange medium at a pressure of 100,000 kPa, volume flow rate of 2000 m3/h and a temperature of 303 K. Water (H_2O) without admixtures was selected as both hot and cold heat exchange medium. The rest of the parameters of this substance are given in the substance data base. The length of the phase contact surface is 10 m, its width is 0.1 m. The heat transfer coefficient is 3600. The results of the heat exchanger computer model are given in Figures 6, b.

The fact that they match the results obtained with the Aspen Hysys software complex proves the adequateness of the implemented heat exchanger model. Unlike its analog, the component implemented in the CPS modeling allows for interactive change of parameters during the simulation experiment.

The dependences for temperature distribution of hot and cold heat-exchange medium plotted in the MARS modeling environment using component circuit method are given in Figure 7.

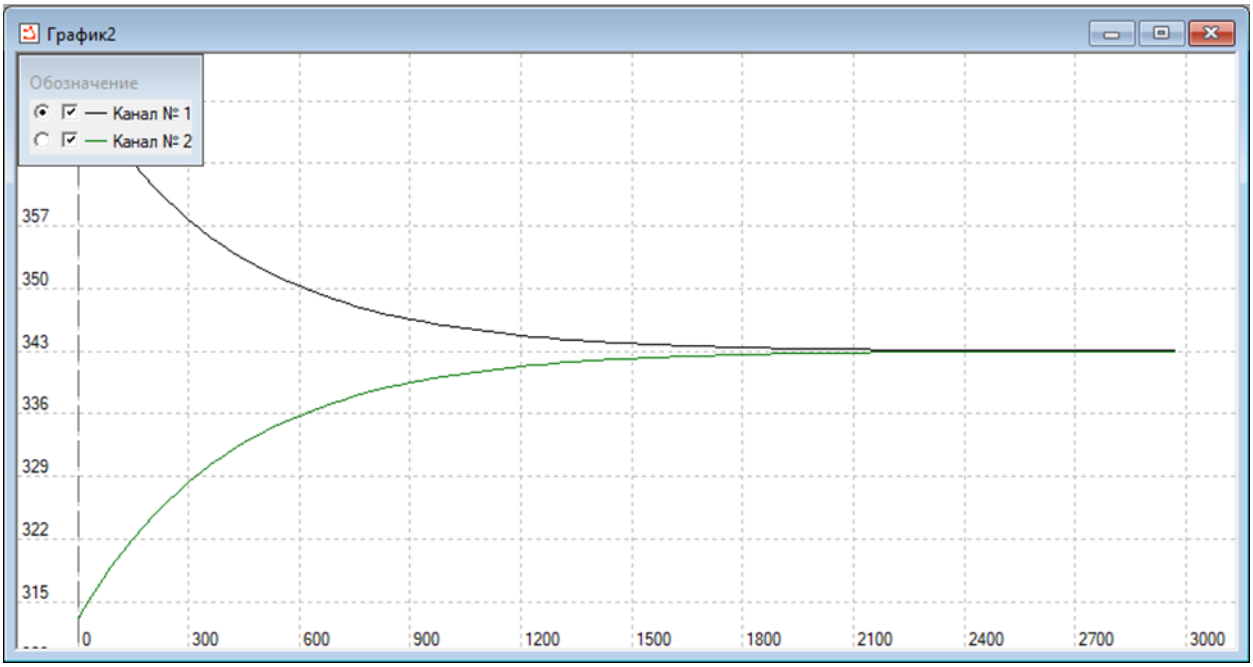

Figure 7. Temperature of hot and cold heat exchange mediums along the length of the heat exchanger

Exponential changes in temperature of hot (black line in Figure 7) and cold (green line in Figure 7) medium confirm the correctness of the implementation of the heat exchanger model with distributed parameters made with the component circuit methods with non-uniform vector couplings. In order to improve the execution speed of the simulation experiment, an algorithm described in [20] was used with the universal computing core.

6. Conclusion

The solution of the CPS research and functional design tasks stated in the paper may be automated by developing a method and software tools for computer modeling of this class of systems. To that end, a proposed generalized structural and functional diagram of a CPS was used to identify parameters and variables of elements and apparatuses. In order to construct models of each of them in the format of the component circuit, a structure of non-uniform vector coupling was suggested and put into the foundation of developing a generalized component of a chemical processing system. It allows describing the processes of transformation of physical variables (hydraulic and thermodynamic) and composition of substances with linear, non-linear, and differential equations with parameters and variables distributed along the

length of the apparatus in question. A heat exchanger component has been implemented on the basis of a generalized CPS component and used to model processes inside the heat exchanger.

The method considered in this paper was implemented in the simulation environment [21] that provides automatic solutions of problems in univariant and multivariant analysis, as well as a parametric synthesis that includes CPS studies and functional design. Currently, this software allows modeling processes taking place inside natural gas processing systems. After certain changes, it will be able to form computer models of process systems in oil processing, and other multicomponent matter flows subject to physical and chemical transformations.

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