Petroleum and Coal

Article **Open Access**

AN ALGORITHM TO IMPROVE THE SPEED AND ACCURACY OF ANALYSIS OF CHEMICAL PROCESS SYSTEMS OPERATION

V. V. Dmitriev[1], T. V. Gandzha[1], I. M. Dolganov[2], Natalia V. Aksenova[2]*

[1] *Tomsk State University of Control Systems and Radio-electronics (Tomsk, Russia)*
[2] *National Research Tomsk Polytechnic University (Tomsk, Russia)*

Received May 2, 2017; Accepted July 10, 2017

Abstract

The paper presents a method to improve the speed of modeling in the MARS modeling framework. The framework allows for flexible modeling of complex processes of chemical industry by representation of industrial apparatuses as sets of primitives in a component circuit. Typical abstract primitives used in modeling of chemical process systems are analyzed: source, mixer, and separator. They are found to often contain variables whose value may be determined separately with less computational load compared to their inclusion into the general system of linear and linearized equations. An algorithm for formation of a shortened system of equations and independent solution of easily solvable equations is presented.

Keywords: chemical technological systems; a mathematical model; computational experiment; objectives of research and functional design.

1. Introduction

Nowadays most of research in chemical process system (CPS) modeling is concentrated in analyzing the process behavior under continuous inputs. There are software models and methods for their analysis being developed which allow to determine hydraulic and thermodynamic characteristics as well as concentration of components in multicomponent material flows between the CPS units**.** They are usually implemented within a certain framework such as ASPEN HYSYS [1], ChemCAD [2-3] and others. Multiple CPS models are also directly implemented in different programming languages [4- 6]. Lacking systemic attributes, they do not allow for fast enough formation and studying of different equipment layouts. Complex changes are usually necessary to adapt the model to a new problem.

When resolving the functional design and operation tasks for the CPS a pressing issue is inclusion of automation elements into the studied CPS model to allow setting and studying of accuracy and dynamic characteristics of instruments and actuating mechanisms. Instruments are principally geared towards measuring hydraulic and thermodynamic characteristics, as well as concentration of components (substances) in the multicomponent material flows. The actuating mechanisms directed by electric signals change the hydraulic and thermodynamic characteristics of the flows that determine speed and accuracy of physical and chemical processes in the CPS units. A complex of the CPSs together with their actuating mechanisms and instruments hereinafter will be called the Controlled Process Object (CPO). Together with the controller, the CPO forms a Complex Controlled Process System (CCPS).

MARS modeling framework [7] is one of the modern universal software solutions for computer modeling of controlled objects and systems. Being founded on the component circuit method, (CCM) [8], it allows for modeling of controlled process and technological objects together with their information, energy and material (including multicomponent) flows represented in links.

Automation of CCPS modeling, where the CPOs are CPSs with their automation elements, opens possibilities for solution of the task to choose optimal instruments and actuating

mechanisms for required accuracy and fast response, as well as for creation of operational algorithms of the controllers in automatic and semi-automatic modes. Besides that, the software solution for computerized CCPS modeling with implemented links to an actual CPO may serve as a basis for smart control systems for CPS processes that transform the multi-component material flows.

Universal computational kernel [9] serves as an algorithmic apparatus for mathematical modeling of non-uniform process units within the MARS framework. It is based on the principle of formation and solution of a system of algebraic differential equations for all the component links variables in the component circuit which serves as a computer model of the object studied within the CCM. This principle introduces redundancy into the system of equations due to the fact that each equation may include one previously undetermined variable. Solution of such a system of equations requires a large number of operations, which may be sequestered by preliminary determination of variables that may be represented explicitly from the CPS mathematical models.

For that end, the mathematical models of the components shall have causative orienting perormed on the input variables with respect to the output variables.

2. Interpretation of the component circuit method for modeling of chemical process systems

The component circuit method [8] is a universal method of computer modeling of complex technical and process objects. Each objects represented in this format shall allow for decomposition into linked elements with flows of information, non-uniform energy flows and multi-component material flows between the elements. For that end, a computer model may be constructed in the CCM format, where each element of the system will be substituted with a component serving as its model and describing the processes therein.

In the CCM format the model of the controlled CPS, hereinafter called a component circuit, is a set of interlinked chemical processing units. Each of them is a physical and chemical system (PCS) [10] that includes processes where multicomponent material flows undergo transformation. The control of the processes inside the PCS is performed by actuating mechanisms, which get signals from the controllers, while the measurement of observed variables and further transmission of values to the controllers is performed by instruments, each of which is associated with a certain component (model of a certain unit or device).

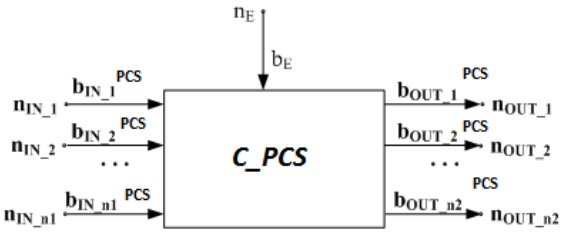

Figure 1. Generalized component of the physical and chemical system

Each PCS unit with the process in it in the CCM format is represented by a component (Fig. 1), whose model is constructed with considerations for four principal aspects:

– *the geometric aspect* creates a provisional graphical and alphabetical reference of the component in the scheme editor of the CPS computer model. It also determines the geometric form and sizing of the unit described by the component which influence the characteristics of the processes inside;

– *the topological aspect* forms the following sets of component links:

– a set of input physical and chemical links

$$S_{IN\_1}^{FChS} = b_{IN\_1}\eta^{-}n_{IN\_1}\ , S_{IN\_2}^{FChS} = b_{IN\_2}\eta^{-}n_{IN\_2}\ ,\ldots, S_{IN\_n1}^{FChS} = b_{IN\_n1}\eta^{-}n_{IN\_n1}\ , \quad (1)$$

to the left of the component, they are the ways by which input material flows come to the component for transformation of their physical characteristics and/or makeup;

– a set of output physical and chemical links

$$S_{OUT\_1}^{FChS} = b_{OUT\_1}\eta^{-}n_{OUT\_1}\ ,S_{OUT\_2}^{FChS} = b_{OUT\_2}\eta^{-}n_{OUT\_2}\ ,. \qquad (2)$$
$$S_{OUT\_n2}^{FChS} = b_{OUT\_n2}\eta^{-}n_{OUT\_n2}$$

They are to the right of the component and are intended for output of the transformed material flows from the PCS component;

– link $S_E = b_E\eta^{\pm}n_E \rightarrow n_E \rightarrow V_{nE}, b_E \rightarrow V_{bE}$ describes the process of supply or extraction of energy of different physical nature, as necessary for or released during the transformation. It is characterized with two variables: potential V_{nE} and flow V_{bE}, whose product for any moment of time defines momentary power of the energy being transferred through this link.

– From the point of view of the *physical aspect,* each link is associated with a set of variables describing the processes inside the component in its mathematical model. Each input (1) and output (2) physical or chemical link, being non-uniform vector values [11], represents a set of two energy links and one uniform vector link

$$S_j^{FChS} = S_j^G, S_j^T, S_j^C \ , \qquad (3)$$

where $S_j^G = b_j^G\eta n_j^G \rightarrow n_j^G \rightarrow P_j, b_j^G \rightarrow G_j$ is the energy link pertaining to hydraulic subaspect of the physical aspect. It is characterized with the following variables: potential P_j is the pressure at the node; flow G_j is the molar flow of the material. Hereinafter such link is called a hydraulic link; $S_j^T = b_j^T\eta n_j^T \rightarrow n_j^T \rightarrow T_j, b_j^T \rightarrow Q_j$ is an energy link of thermodynamic subaspect of the physical aspect, characterizing the store of thermal energy in the material flow. It includes the following variables: potential T_j *(*temperature), flow Q_j *(*thermal flow); $S_j^C = b_j^C\eta\mathbf{n_j^C} \rightarrow \mathbf{n_j^C} \rightarrow \mathbf{C_j}, b_j^C \rightarrow \varnothing$ – a uniform vector link with a variable vector $\mathbf{C_j}$, characterizing the material concentrations in the link being described. Its dimensionality corresponds to the number of substances circulating inside the entire CPS.

According to the physical aspect, each variable of each link has to be unique in the physical component basis.

– From the point of view of the *mathematical aspect* the processes in any component of the PCS are to be described with a system of equations constructed for variables of all the links of this component. They will form a vector, called the solution vector of the component

$$V_{K\_FChS} = \left[\mathbf{P_K} \quad \mathbf{G_K} \quad \mathbf{T_K} \quad \mathbf{Q_K} \quad \mathbf{C_K}\right]^T \qquad (4)$$

where $\mathbf{P_K}$ is the pressure vector for all the nodes formed by connection of component links to the links of other components; $\mathbf{G_K}$ is the material flow vector covering all its input and output streams; $\mathbf{T_K}$ is the temperature vector of the material flows; $\mathbf{Q_K}$ is the thermal flows vector; $\mathbf{C_K}$ is the concentration vector for input and output streams of the PCS component.

The mathematical model of a component includes equations of the following types [8]:

– linear equations

$$\sum_i a_i \cdot V_i = b \ , \qquad (5)$$

where a_i, b are constant coefficients; V_i are link variables which are parts of the solution vector of the component (4);

– non-linear equations

$$f\left(V_{K\_FChS}\right) = 0 \ , \qquad (6)$$

where $f\left(V_{K\_FChS}\right)$ is a non-linear function;

– ordinary differential equations

$$\frac{d\Psi\ V_{K\_FChS}}{dt} = f\ V_{K\_FChS}, t \quad , \tag{7}$$

where $\Psi\ V_{K\_FChS} = \sum_i \psi_i \cdot V_i$ is a linear form with respect to the link variables of the component (4), $f\ V_{K\_FChS}, t$ is an arbitrary function.

– source equations

$$\sum_i a_i \cdot V_i = b\ t \tag{8}$$

where a_i are constant coefficients; $b\ t$ is an arbitrary function of time.

Left parts of linear (5) and non-linear equations (6), as well as the right parts of differential equations (7) may include not only vector variables V_{K_FChS}, but their partial derivatives with respect to geometric sizes of the modeled CPS unit $\frac{\partial V_{K\_FChS}}{\partial l}$. In such a case this equation will come under the class of linear, non-linear or differential equations with partial derivatives.

A Component circuit, which is a computer model of the studied object or system within the CCM framework is generally an arbitrary set of interlinked components, whose links (*branches)* are connected in common points, which are called *circuit nodes*. Formally, a component circuit is a collection of three sets

$$C=(K,B,N) \tag{9}$$

where *K* is a set of components; *B* is a set of links (branches); *N* is a set of component circuit nodes, formed by commutation of the component links *S*.

Each link S_j of a component in *K* (1) with the number b_j, which is the number of its branch, given in the local coordinate basis of the component, is associated with a number B_J, unique for the component circuit *C*, where *J*=1..*CB, CB* is the number of branches in this circuit.

Connection of links *B* of the components in the set *K* results in nodes of the set *N*. In each of them, the following two topological laws are valid:

– the law of equality of all the potential variables of the links pertaining to a single subaspect of the physical aspect;

– the law of equality to zero of the sum of flow variables of a single subaspect of the physical aspect of all the links having connection to the same node.

Construction of the component circuit mathematical model of the CPS involves uniting computational models of the components M_{Ki} and node topological laws M_{Nk} for potential and flow variables

$$M_C = \left[\bigcup_i M_{Ki} \cup \bigcup_k M_{Nk} \right]. \tag{10}$$

As per the first topological law, the potential variables of a single subaspect of the physical aspect connected to the same node are associated with one number in the global coordinate basis of the circuit. From the second topological law, for each node the topological equations are formed looking like

$$\sum_i \alpha_i \cdot V_{Bi} = 0 \quad , \tag{11}$$

where α_i is the numeric coefficient which is +1 if the flow B_i directed towards the node, -1 if it is directed from the node, and 0 if the branch B_i is not connected to the node for which the equation (11) is being formed.

The complex of topological and component equations (10) allows for determination of all the values of the link variables of the circuit in question, comprising its solution vector

$$V = \left[V_N \ \ V_B \right]. \tag{12}$$

The solution vectors of each of the PCS components, which are used to generate the solution vector of the whole circuit (12), will contain three types of variables

$$V^K = \left[V_{IN}^K, V_{OUT\_1}^K, V_{OUT\_2}^K\right], \quad (13)$$

where V_{IN}^K is the set of input link variables of the component; $V_{OUT\_1}^K$ is the group of variables, allowing their explicit determination directly inside the component models; $V_{OUT\_2}^K$ is an aggregate of variables not allowing for their explicit representation in the models of respective components.

To minimize the computational procedures implemented in the universal computation kernel for creation, linearization and solution of the system of algebraic and differential equations there is an algorithm which determines the values of variables of the set $V_{OUT\_1}^K$ (13) directly inside the components in cases where values of parameters V_{IN}^K are determined beforehand and introduced into the relevant components of the solution vector of the circuit (12). To find the values of variables pertaining to the set $V_{OUT\_2}^K$ equations are formed and added to the system of equations, where solution determines the relevant values.

The interpretation of the CCM considered above allows for creation of computer models of principal elements and units of chemical industry with possible explicit determination of values of variables if they allow for calculation directly inside the component.

3. Component set of components of chemical process systems and classification of its models

Source of mixture, represented in Figure 2, is a point of supply of a multicomponent material flow into the CPS. It has the only link $S_1 = b_1 \eta n_1 \rightarrow P_1, G_1, T_1, Q_1, \mathbf{C_1}$ where P_1 is the pressure in the node n_1, G_1 is volumetric flow of the multicomponent mixture in the stream formed by the branch b_1, T_1 is the temperature in the node n_1; Q_1 is the thermal flow in the stream of the branch b_1, $\mathbf{C_1}$ is the concentration vector for the substances comprising the multicomponent stream. The following parameters and characteristics are set up in the component's options: P^{DEF} is the value of pressure at the node n_1; G^{DEF} is the value of volumetric flow of the multicomponent mixture in the branch b_1; T^{DEF} is the value of pressure at the node n_1; N_C is the number of components (substances) forming the multicomponent material flow; **Names** is a set of substance names, each of them corresponding to a parameter line in the flow component data base; $\mathbf{C}^{\mathrm{DEF}}$ is the concentration vector of the components that form the multicomponent material flow.

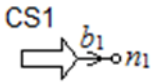

Figure 2. Component source of mixture

The mathematical model of the Source of Mixture component includes the following equations

$$\begin{aligned} P_1 &= P^{\mathrm{DEF}} \\ G_1 &= G^{\mathrm{DEF}} \\ T_1 &= T^{\mathrm{DEF}} \\ Q_1 &= Q^{\mathrm{DEF}} \\ C_{1i} &= C_{1i}^{\mathrm{DEF}}, \end{aligned} \quad (14)$$

where $Q^{\text{зад}}$ is the thermal flow calculated with the formula

$$Q^{\text{DEF}} = G \cdot T \cdot \sum_{i=1}^{N_C} \rho_i \cdot CP_i \cdot C_i^{\text{DEF}\ 2}, \quad (15)$$

where ρ_i is the density of the substance $Name_i$, selected from the component database by the substance name; CP_i – heat capacity of the substance which is the function of its temperature T

$$CP_i = CPVAP\_A_i + CPVAP\_B_i \cdot T + CPVAP\_C_i \cdot T^2 + CPVAP\_D_i \cdot T^3, \quad (16)$$

where $CPVAP\_A_i, CPVAP\_B_i, CPVAP\_C_i, CPVAP\_D_i$ are constants in the equation of ideal gas density where CP is given in cal/(mol*K). These constants are set for each substance in the relevant field of the flow component database [12].

The variables of the only link of the source-type components are in the set $V_{OUT\_1}^K$. Their values may be directly added to the relevant components of the circuit solution (12) inside the component without adding equations (14) to the common system of equations.

Mixers are used to mix two multicomponent flow in chemical processes. Two streams of differing molar flow rate, pressure and temperature progress to this apparatus. The mixer component shown in Figure 3 has two input links $S_1 = b_1 \eta n_1 \rightarrow P_1, G_1, T_1, Q_1, \mathbf{C_1}$, $S_2 = b_2 \eta n_2 \rightarrow P_2, G_2, T_2, Q_2, \mathbf{C_2}$ and one output link $S_3 = b_3 \eta n_3 \rightarrow P_3, G_3, T_3, Q_3, \mathbf{C_3}$

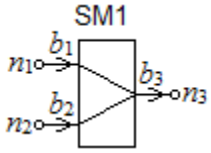

Figure 3. Mixer component

The mathematical model describing the mixing of two multicomponent flows is described by a system of equations

$$\begin{aligned} &P_1 + P_2 - P_3 = 0 \\ &G_1 + G_2 - G_3 = 0 \\ &G_1 \cdot T_1 + G_2 \cdot T_2 - G_3 \cdot T_3 = 0 \\ &Q_1 \cdot T_1 + Q_2 \cdot T_2 - Q_3 \cdot T_3 = 0 \\ &C_{1i} \cdot G_1 + C_{2i} \cdot G_2 - C_{3i} \cdot G_3 = 0 \end{aligned} \quad (17)$$

The set of input variables of the mixer component includes the following variables $V_{IN}^K = P_1, G_1, T_1, Q_1, \mathbf{C_1}, P_2, G_2, T_2, Q_2, \mathbf{C_2}$. Each equation of the model (17) includes only one variable of one of the output links. If each input link variable S_1, S_2 is defined during creation of the mathematical model of the mixer component, then each variable of the only output link of the component S_3 may be expressed in the explicit form from the relevant equation of the system (17)

$$\begin{aligned} &P_3 = P_1 + P_2 \\ &G_3 = G_1 + G_2 \\ &T_3 = \frac{G_1 \cdot T_1 + G_2 \cdot T_2}{G_3} \\ &Q_3 = \frac{Q_1 \cdot T_1 + Q_2 \cdot T_2}{T_3} \\ &C_{3i} = \frac{G_1 \cdot C_{1i} + G_2 \cdot C_{2i}}{G_3} \end{aligned} \quad (18)$$

.

In this case its value will be calculated from formulas (18) and the equation from the system (17) containing this variable will not be added to the common system of equations.

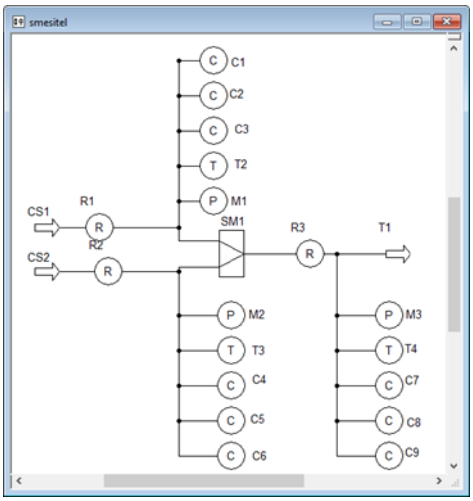

Fig. 4. Computer model of the mixing section of two material flows

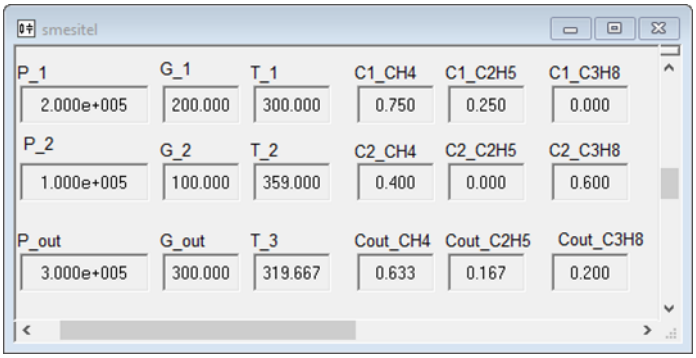

Figure 5. Results of analysis of the computer model of the mixing section for two material flows

Figure 4 shows an example of a model of the mixing section of two material flows in gaseous phase. Mixture of methane and propane with the ratio of 0.75: 0.25 is supplied to the mixer from the source SC1 at the speed of 200 mol/sec with pressure P=200 kPa and temperature of 300 K. The source SC2 with pressure 100 kPa and speed of 100 mol/sec supplies a mixture of methane and ethane with the ratio of 0.4: 0.6 at the temperature of 350K.

Figure 5 shows the results of analysis of the mixing section for two material flows.

Heat exchanger is an apparatus of chemical process system where exchange of heat happens between two heat transfer agents, which are multicomponent material flows in gaseous or liquid state having different temperature. The heat is transferred from the more heated (hereinafter - hot) agent to the less heated (hereinafter - cold) through a separating wall. Taking into account that the heat exchange happens along the whole length of the rectangular heat exchanger, changes in temperature of hot and cold medium are described by a system of differential equations in partial derivatives along the length of the heat exchanger [13]

$$\frac{\partial T^H}{\partial l} = \frac{K \cdot d}{G^H \cdot CP^H\ T^H\ l\ \cdot \rho^H} \cdot\ T^H\ l\ - T^C\ l$$

$$\frac{\partial T^C}{\partial l} = -\frac{K \cdot d}{G^C \cdot CP^C\ T^C\ l\ \cdot \rho^C} \cdot\ T^H\ l\ - T^C\ l \qquad (17)$$

,

where K is the heat transfer coefficient; d is the width of the separating wall area; G^H, G^C are molar flow rates of hot and cold heat transfer mediums; ρ^G, ρ^C are density values of hot and cold heat transfer medium respectively; CP^H, CP^C are specific molar thermal conductivity values of the mediums calculated per formula [12]

$$CP\ T\ = \sum_{i=1}^{N_C} CP_i\ T\ \cdot C_i \qquad (18)$$

,

where CP_i are specific thermal conductivity values for the substances in the medium in question; C_i are concentration values for this medium.

Changes in thermal flows of hot and cold heat transfer mediums respectively along the entire length of separating wall is described with the following equations

$$Q^H(0)-Q^H(L)=\rho^H\cdot G^H\cdot\left(CP^H\left(T^H(L)\right)\cdot T^H(L)-CP^H\left(T^H(0)\right)\cdot T^H(0)\right)$$
$$Q^C(0)-Q^C(L)=\rho^C\cdot G^C\cdot\left(CP^C\left(T^C(L)\right)\cdot T^C(L)-CP^C\left(T^C(0)\right)\cdot T^C(0)\right) \quad (19)$$

The Heat Exchanger component implemented on the basis of equations (15)–(17) is shown in Figure 6. It has the following links:

– $S_1=b_1\eta^- n_1 \rightarrow P^H\ 0\ ,G^H\ 0\ ,T^H\ 0\ ,Q^H\ 0\ C^H\ 0$ is a link supplying hot heating medium to the heat exchanger;

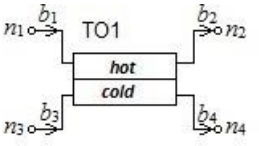

Figure 6. Heat exchanger component

– $S_2=b_2\eta^- n_2 \rightarrow P_2^H\ L\ ,G_2^H\ L\ ,T^H\ L\ ,Q^H\ L\ ,C_2^H\ L$ is a link by which the hot heating medium leaves the apparatus;

– $S_3=b_3\eta^- n_3 \rightarrow P_1^C\ 0\ ,G_1^C\ 0\ ,T^C\ 0\ ,Q^C\ 0\ ,C_1^C\ 0$ is a link supplying cold heating medium to the heat exchanger;

– $S_4=b_4\eta^- n_4 \rightarrow P_2^C\ L\ ,G_2^C\ L\ ,T^C\ L\ ,Q^C\ L\ ,C_2^C\ L$ is a link reflecting release of cold heating medium from the heat exchanger.

Let us break the entire length of the heat exchanger L into a number of segments Δl, where heat exchange rate is constant over the length of the segment. Application of the explicit Euler scheme for each of the differential equations (15) gives the algebraic form:

$$\begin{aligned}
&G^H(0)\cdot CT\left(T^H(l+\Delta l)\right)\cdot T^H(l+\Delta l)-(1-K\cdot d\cdot\Delta l)\cdot T^H(l)-K\cdot d\cdot\Delta l\cdot T^C(l)=0\\
&G^C(0)\cdot CT\left(T^C(l+\Delta l)\right)\cdot T^C(l+\Delta l)-(1-K\cdot d\cdot\Delta l)\cdot T^C(l)+K\cdot d\cdot\Delta l\cdot T^H(l)=0\\
&Q^H(0)-Q^H(L)-\rho^H\cdot G^H(0)\cdot\left(CP^H\left(T^H(L)\right)\cdot T^H(L)-CP^H\left(T^H(0)\right)\cdot T^H(0)\right)=0\\
&Q^C(0)-Q^C(L)-\rho^C\cdot G^C(0)\cdot\left(CP^C\left(T^C(L)\right)\cdot T^C(L)-CP^C\left(T^C(0)\right)\cdot T^C(0)\right)=0\\
&P^H(0)-P^H(L)=0\\
&G^H(0)-G^H(L)=0\\
&C_i^H(0)-C_i^H(L)=0\\
&P^C(0)-P^C(L)=0\\
&G^C(0)-G^C(L)=0\\
&C_i^C(0)-C_i^C(L)=0
\end{aligned} \quad (20)$$

The heat exchanger model (20) may simultaneously describe a real apparatus with opposite or in-trail flow of the heat exchange mediums. Its first two equations are constructed for each segment of the apparatus which are obtained in algebraization of the differential equations (17), describing the distributed heat exchange process. Such equations cannot be presented explicitly, because they simultaneously contain variables characterizing the conditions of both heat exchange mediums. Each of the rest of the equations will have one determined variable whose value may be determined only by explicit solution.

The first two equations of the system (20) are composed for each segment into which the length of the heat exchanger is divided for linearization of the differential equations (19). Thus, no equation of the heat exchanger model cannot be solved in its explicit form because the direction of the heating medium streams is not known beforehand for the apparatus being modeled.

Figure 7 shows a computer model of the heat exchanger where a source SC1 supplies hot heat exchange medium with pressure of 100000 kPa, volumetric flow rate of 2000 m3/h and temperature of 363 K. The cold heat exchange medium is supplied by the source SC2 at the pressure of 100000 kPa, volumetric flow rate of 2000 m3/h and temperature or 303K. Demineralized water (H2O) was selected as a heat exchange medium. The rest of the parameters of this substance is given in the substance data base. The length of the contact surface is 10 m, the width is 0.1 m. Heat transfer coefficient is 3600. The results obtained from analysis of the computer model of the heat exchanger are shown in Figures 7 b.

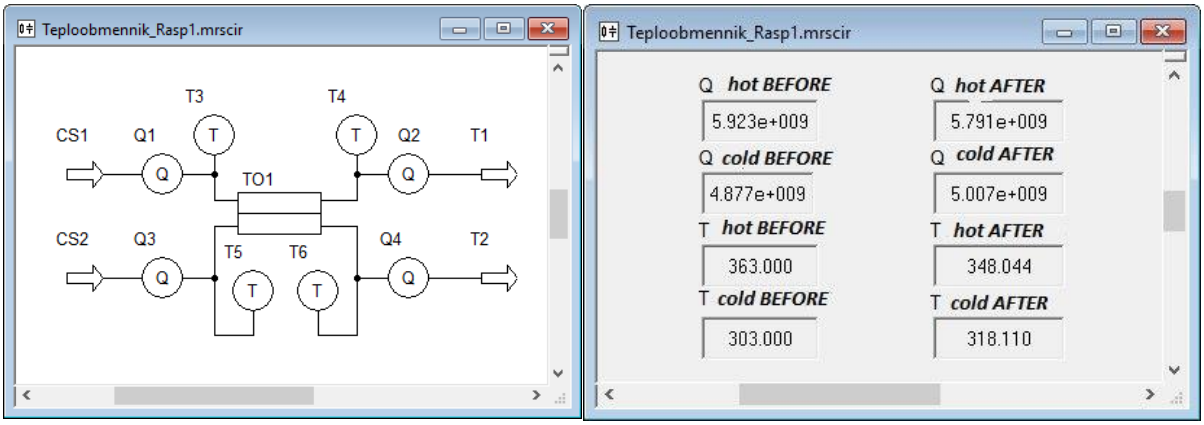

Figure 7. Modeling a heat exchanger. a) computer model of a heat exchanger; b) results of the modeling

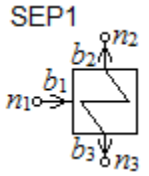

Figure 8. Separator component

Separator is a chemical process apparatus where a gas-liquid mixture is phase separated depending on input parameters. The Separator component shown in Figure 8 was developed for description of the separation process at different values of pressure and temperature. It has the following links $S_1 = b_1\eta^- n_1 \rightarrow P_{In}, G_{In}, T_{In}, Q_{In}, \mathbf{C_{In}}$

– is an input link by which a gas-liquid mixture is supplied to the separator at a certain pressure P_{In} and temperature T_{In};

– $S_2 = b_2\eta^+ n_2 \rightarrow P_G, G_G, T_G, Q_G, \mathbf{C_G}$ is an output link for removal of gas at pressure P_G and temperature T_G from the separator. The blend composition of the gas is represented with a concentration vector $\mathbf{C_G}$;

$S_3 = b_3\eta^+ n_3 \rightarrow P_L, G_L, T_L, Q_L, \mathbf{C_L}$ is an output link for removal of liquid at pressure P_L and temperature T_L. The vector $\mathbf{C_L}$ contains concentrations of substances comprising a given stream.

The mathematical model of the Separator component is a system of equations in the link variable form:

$$
\begin{aligned}
&P_G - P_{In} = 0\\
&P_L - P_{In} = 0\\
&G_{In} - G_G - G_L = 0\\
&e \cdot G_G - G_L = 0\\
&T_G - T_{In} = 0\\
&T_L - T_{In} = 0\\
&Q_G - Q_{In} = 0\\
&Q_L - Q_{In} = 0\\
&C_{In\_i} - e \cdot C_{G\_i} - 1 - e \cdot C_{L\_i} = 0\\
&C_{G\_i} - K_i \cdot C_{L\_i} = 0
\end{aligned}
\qquad (21)
$$

where $i = \overline{1,CF}$ is a number of components (substances) in the input stream of the separator; e is the steam ratio calculated by the golden rule to minimize the target function

$$F\ e = \sum_{i=1}^{CF} C_{In\_i} \cdot \frac{K_i - 1}{1 + e \cdot K_i - 1} \qquad (22)$$

K_i are phase equilibrium constants for the vapor-liquid system calculated from the Soave modification of Redlich-Kwong equation [14].

Taking into account that the input variable vector of the separator model includes the following variables

$$V_{IN} = P_{IN}, G_{IN}, T_{IN}, Q_{IN}, \mathbf{C_{IN}}^T, \qquad (23)$$

each variable of both output links S_2 and S_3 may be expressed explicitly from the relevant equation of the system (21)

$$
\begin{aligned}
&P_L = P_{In}\\
&G_L = e \cdot G_G\\
&T_L = T_{In}\\
&Q_L = Q_{In}\\
&C_{L\_i} = \frac{C_{In\_i}}{K_i \cdot e + 1 - e}\\
&P_G = P_{In}\\
&G_G = \frac{G_{In}}{1 + e}\\
&T_G = T_{In}\\
&Q_G = Q_{In}\\
&C_{G\_i} = K_i \cdot C_{L\_i}
\end{aligned}
\qquad (24)
$$

Figure 9 shows a model of a low-temperature separation section for a gas-liquid mixture at the temperature of -80^{0}C, supplied to the separator input at the pressure of 2 MPa at the rate of 10^7 mol/sec. It has the following blend composition: methane – 0.7812; ethane – 0.03; propane – 0.02; isobutane – 0.0048; n-butane – 0.001; nitrogen – 0.163. The results of the modeling are given in Figures 9a and b.

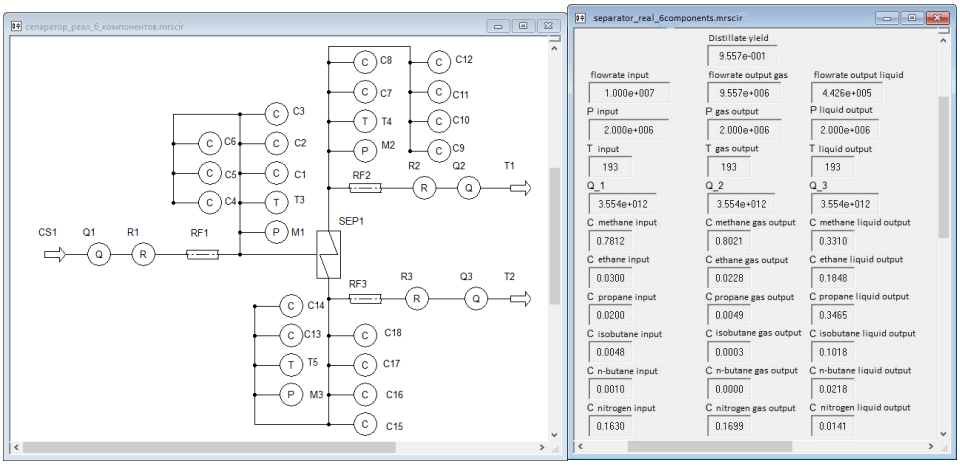

Fig. 9. Computer modeling of a low-temperature separation of natural gas. a) computer model of the section; b) results of the modeling

Analysis of the models of the physical and chemical system shown above with the mathematical apparatus of the universal computational kernel [9] of the MARS framework is redundant, because according to its algorithm it performs formation and solution of all the systems of equation, including the topological and component equations composed for all the component link variables in the analyzed component circuit of the CPS. Use of computational model packing algorithm based on the cause-and-effect analysis of the components is recommended to improve the speed of analysis.

4. Algorithm to form a packed computational model of the CPS by means of the universal computational kernel

The algorithm for formation of the packed computational model of the analyzed chemical process system assumes determination of querying order for the component computational units from sources to terminals while forming the component equations. At that each linear and non-linear equation formed will be checked for possibility of direct calculation of its sole variable. To implement the algorithm in addition to the circuit solution vector (12) a solution flag vector is introduced

$$D = \left[D_N \quad D_B \right]. \tag{25}$$

Each element of the vector D (25) $D_j = \text{TRUE}$ ($j = CN + CB$, where CN is the number of potential variables, CB is the number of flow variables of the studied circuit), if the corresponding element V_j of the vector V (12) is defined at this iteration at the stage of formation of topological and component equations.

Creation of packed computational model of the CPS is implemented in the universal computational kernel [9] and it is assumed that the components form each of the equations in the form of the structure

$$Eq = KL, IB, m2, m3, W \tag{26}$$

where KL is the equation attribute (10-12 – linear with constant or variable coefficients and right parts; 13 – non-linear equations, 14-21 – different types of regular differential equations with linear and non-linear right parts. Differential equations in partial derivatives are solved according to Euler's non-explicit scheme when forming the software model of the component); IB is the number of the variables in the equation; $m2$ is an array of variable numbers (for regular derivatives a code attribute is added to the number); $m3$ is an array of coefficients; W is the absolute term of the equation.

If during the formation of a component equation (26) only one previously undefined variable is introduced, then, this equation is automatically solved for this variable with number j as per the following formula

$$V_{m2\,j} = \frac{W}{m3_j} - \sum_{\substack{i=0 \\ i \neq j}}^{IB} \frac{m3_i}{m3_j} \cdot V_{m2\,i} \qquad (27)$$

.

The formation algorithm for the packed computational model of the CPS where the sources of multicomponent material flows are determined by values of potential and flow link variables of the source consists of the following stages:

1. Formation of a topological array m1 from all the components of the studied circuit, containing the topological pairs

$$T = \pm B_j, N_j \qquad (28)$$

where B_j is the branch number given in the global coordinate basis of the circuit. It assumes the plus sign if the branch is oriented from the branch to the component and minus sign if it is oriented in the opposite direction.

2. Sorting of the components in accordance with their flow direction on the basis of the topological pairs (28). It is performed for output topological pairs containing a branch number with the minus sign. During the sorting the components comprising the studied CPS circuit and shown in Figure 10 as the tree nodes shall be sorted for querying their computational units in the order shown in Figure 10. In the tree nodes there are index numbers showing the querying order for the component computational units.

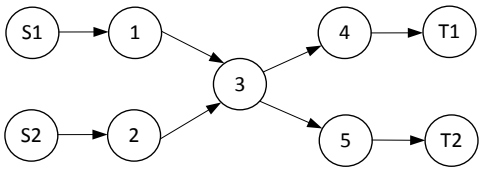

Figure 10. The component sorting rule for computational unit querying

3. Querying computational units of single-link source components S1, S2,…, T1, T2. Such components form the equations of the type (26) with $IB=1$, thus, at the pre-formation stage of the equations from the local coordinates to the global ones direct determination of the relevant variables takes place. In this case their values are directly recorded into the solution vector (12), while corresponding vector members D (25) take the value of TRUE.
4. Formation of topological equations from the topological pairs array (28).
5. Explicit solution of the topological equations which were formed at stage 4, using the formula (27).
6. Stage 5 is performed until there are no more solvable equations. The solved equation is removed from the system of equations. Unsolved equations stay in the system for later solution.
7. Querying of computational units of the components is performed in the order set in Figure 10 while trying to directly solve each linear and non-linear equation with the formula (27). For each differential equation directly from the component the relevant procedure is called which is included under the class of linearization methods for linear equations and algebraization of differential equations *CFormirEquation*, with considerations for its possible solution with the formula (27). The solved equations are removed.
8. For the remaining system of linear algebraic equations, if there are at least two equations a solution method is called to determine the values of previously unresolved variables. This system of equations will contain the previously unsolved equations.
9. The results which are subject to visualization are selected from the circuit solution vector (12) during the querying of the component measurement unit and are transmitted to the visualization unit [15], which together with the interactive control of parameters forms a set of visual tools and instruments within the MARS modeling framework.

The algorithm allows to reduce the size of the system being solved with the linear algebra algorithms by using direct determination of a number of variables in the circuit. It also allows to minimize the time spent analyzing circuits which allow for explicit solution for a number of circuit link variables.

5. Conclusion

This paper considered a numerical algorithm providing improved speed and accuracy of CPS analysis by algorithms of the universal computational kernel of the MARS multilevel computer modeling framework. It is based upon direct computation of the values of variables which are limited to a single equation with a previously undefined single variable. The remainning equations form a system of linear and linearized equations solved with the linear algebra algorithms involving a large number of elementary operations.

The proposed algorithm of explicit-implicit analysis of CPS computer models allows reducing the time spent solving the modeling task by 25-50 % in comparison to implicit methods which were previously implemented in the universal computational kernel of the MARS multilevel computer modeling framework.

References

[1] Kuznetsov OA. Basic Operation of Aspen HYSYS: A Learning Guide, Direkt Media, 2015; 153 pp.
[2] Mathematical Modeling of Chemical Process Systems With the Help of ChemCad Software: A Learning Guide / Kazan State University of Technology. Ed.: Ziatdinov NN, Lapteva TV, Ryzhov DA, Kazan, 2008; 160 pp.
[3] CHEMCAD Suite [Electronic resourse] – Access mode: http://www.chemcad.co.uk/, free. (Accessed on 30.01.2015).
[4] Stroustrup B. The C++ Programming Language. Special Edition, Moscow, Binom, 2011; 1136 pp.
[5] Gryzlov VI, Gryzlova TP. Turbo Pascal 7.0, Moscow, DMK, 2000; 416 pp.
[6] Pilschikov VN. Assembler. Programming with IBM PC Assembler Language, Moscow: Dialog-MIFI, 1999; 288 pp.
[7] MARS – an environment for modeling of technical objects and systems. A Monograph /Dmitriev VM, Shutenkov AV, Zaychenko TN, Gandzha TV. Tomsk: V-Spektr, 2011; 278 pp.
[8] Dmitriev VM. Industrial robots modeling automation /Dmitriev BM, Arays LF, Shutenkov, AV. Moscow, Mashinostroyenie, 1995; 304 pp.
[9] Dmitriev VM, Shutenkov AV, Gandzha TV. Architecture of the universal computing kernel for the realization of virtual laboratories. Pribory I Sistemy Upravleniya, 2004, 2: 24 - 28.
[10] Kafarov VV. Systemic Analysis of Chemical Technology. A Topological Analysis of Formalization / V.V. Kafarov, I.N. Dorofov, Moscow, Nauka: 1979; 304 pp.
[11] Dmitriev VM. Building Principles for Modelling Complex Technological Facilities with Non-Uniform Vector Links / V.M. Dmitriev, T.V. Gandzha, S.K. Vazhenin. Modern Technologies. Systemic Analysis. Modeling, 2014, 1: 104-111.
[12] Reid R, Prausnitz J, Sherwood T. The Properties of Gases and Liquids: A Reference. (Russian Edition). – 3rd Edition, updated and revised, Leningrad, Khimia, 1982; 592 pp.
[13] Dytnerskiy YuI. Processes and Vessels of Chemical Technology: A textbook for institutions of higher education. 2nd edition. In 2 volumes: Part 1. Theoretical Foundations of Chemical Processes. Hydromechanical and Thermal Processes and Vessels, Moscow, Khimia: 1995; 400 pp.
[14] Akberov RR. Specific Features in Calculation of Vapor-Liquid Phase Equilibrium for Multicomponent Systems With The Help of Soave Modification of Redlich-Kwong Equation. Theoretical Foundations of Chemical Technology, 2011, 45(3): 329 - 335.
[15] Dmitriev VM, Gandzha TV, Gandzha VV, Panov SA. Computer simulation of the visual interface in virtual instruments and devices. Scientific Visualization, 2016, 8(3): 111 - 131.

To whom correspondence should be addressed. Department of foreign languages of the Institute of Cybernetics, Tomsk Polytechnic University, 30, Lenin Avenue, Tomsk, 634050, Russia; tel.: (+7-923)4577428, E-mail: polozova15@tpu.ru