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DEVELOPMENT OF A TECHNOLOGICAL MODELING SYSTEM FOR REFINING PROCESSES

Siddikov I.Kh., Ganiev A.A.

Annotation. The article considers with the creation of a modeling system that allows the formation the dynamics of the technological process. Taking into account its physical and chemical properties. To solve this issue, the application of a semantic network is proposed, which ensures the aggregation of process models based on their compatibility. The proposed approach is implemented for dehydrogenation parameters, which showed the effectiveness of the proposed approach.

Key words: refining, modeling, neural network, semantic network.

Introduction: The current state of the oil refining industry is characterized by the need for a constant increase in the efficiency of production, which, in turn, makes great demands on the means of automation, control and management of various levels. This applies to both automated control systems for technological process parameters and information technologies designed to predict the performance of installations and the quality of commercial products. The software of foreign manufacturers is intended mainly for the processes of preparation and transportation of oil and gas and, as a rule, is not suitable for calculating reactor processes for the catalytic processing of hydrocarbons. Existing developments are intended to solve the problems of collecting, archiving and structuring information by local databases and database management systems.

Technological modeling systems for oil refining and petrochemical processes have distinctive properties that make it possible to more effectively solve the problems of monitoring and optimizing oil refineries. The innovativeness of the method lies in taking into account the reactivity of hydrocarbons of multicomponent feedstock, the potential of the catalyst, and the nonstationarity of reactions on the catalyst surface. This approach makes it possible to improve technologies, assess the condition of catalysts, optimize processes, and monitor and forecast production. Under such systems are introduced into production, the problem arises of synthesizing them with an automatic process control system (APCS) of the plant.

Existing process control systems solved the problems of collecting, archiving, structuring information and providing it to users, which include a large number of distributed control systems and communication servers that perform the functions of transferring technological information between control levels.

However, providing only technological information does not create a complete image of the operation of the enterprise. It is necessary to correlate these data with others, therefore the next step in the development of process control systems at refineries is the analytical processing of the data obtained.

Main part

For analysing the state of technological objects and on the basis of this forecasting of production, it is necessary to have technological modeling systems that use arrays of information from technological monitoring.

Under developing a modeling system, it becomes necessary to synthesize a mathematical description of a chemical technological system (CHTS). The essence of the hierarchical principle of synthesis of a mathematical description lies in the fact that the mathematical description of each subsequent structural level should be included as the main part in the mathematical description of the last level.

The creation and improvement of modeling algorithms is associated with solving a number of complex problems in defining goals and objectives, developing and making managerial decisions. The fundamental issue here is the choice of a mathematical base, since the automation of the study of structurally complex dynamical systems is associated with a set of manifestations of the features of modeling, analysis and synthesis of the considered classes of systems. One of the possible promising ways to solve this problem is to create problem-oriented modeling systems in which models are extracted from elementary operations given in the form of ratios.

The basis of modeling systems hierarchical description of the dynamics of the system under study, represented by a family of models, each of which describes the behavior of a dynamical system from the point of view of various levels of abstraction.

With regard to the problems being solved, it is proposed to distinguish two directions of hierarchical models:

- a hierarchy along the vertical, in which the division of models by levels is carried out according to the structural and functional features of the system;
- a horizontal hierarchy, in which the division of models by levels is carried out depending on the research methods.

Three levels of models are distinguished vertically in the hierarchy:

- the level of basic models containing the simplest models;
- the level of local models, displaying the structural and functional properties of functionally complete devices focused on solving particular problems;
- the level of global models that reflect the organizational characteristics of systems and the models with a high degree of detail.

The horizontal hierarchy includes four levels of models, depending on the methods of their study:
- models that allow obtaining the results of calculating processes based on analytical modeling;
- models reflecting the discrete nature of processes and representable by a logical-differential equation;
- models displaying the structural conjugation of mathematical schemes of processes based on neural network algorithms;
- models that allow it to optimize and predict the state of the system based on artificial intelligence methods.

In the general case, the design process involves the development of a set of models that form a multilevel structure and reflect the iterative, dynamic and hierarchical nature of the processes under consideration.

For presenting knowledge, a semantic network is used, the objects of which are variables called computational models associated with private relations. Semantic memory (SM) is an image of a subject area (SA). It stores all the information (knowledge) that determines the functions of the system. Algorithms and special knowledge about the admissible properties of classes of algorithms are represented in the SP in the form of semantic models, which allow generating a modeling algorithm, processing and its execution.

Mathematical models of objects for modeling are stored in the joint venture in the form of a set of relations, which can also be changed and supplemented. As a result, the user gets the opportunity to correct the semantics of the algorithms, set various criteria for admissibility, introduce new algorithms and models, and correct the object model.

Formally, modeling algorithms based on these models can be presented in the following form:

\[ \mathbf{M} = \{ I, \Phi, X, Y, \Omega \} \]

where \( I \) - model identifier; \( \Phi = P \) (\( x_1, x_2, \ldots, x_n \)) - a unary predicate defined on the set \( X \). The meaning of this predicate is to formally determine the possibility of using this model; \( \Phi: X Y (XUY = Z) \) - maps describing a set of properties of the modeling algorithm; \( X = \{ x_1, x_2, \ldots, x_n \} \) - input variables of the computational model; \( Y = \{ y_1, y_2, \ldots, y_n \} \) - output variables of the computational model; - set of variables; \( Z = \{ z_1, z_2, \ldots, z_n \} \) - the area of application of the model, which is set by a pair of areas of definition \( X \) and \( Y \) values, i.e. \( \Omega = \{ X, Y \} \)

In the process of working with models, there may be two types of input variables:
- definite and indefinite. In accordance with this, the sets \( X \) will be divided into two disjoint subsets \( \mathbb{X} \) and \( \mathbb{X} \), i.e.

\[ \mathbb{X} \cap \mathbb{X} = \emptyset \]

Elements of the set \( \mathbb{X} \) can be determined with the introduction of one or another relationship between certain variables \( \mathbb{X} \). Such a connection leads to the formation of more complex multilevel computational models, or otherwise, the model \( \mathbb{M} \), which has an output the vector \( Y \) and indefinite vectors of variables \( \mathbb{X} \), can be represented as a set of \( N_m = N_i \cup \mathbb{X} \) models of vector \( Y \), \( k = 1, 2, \ldots, N_m \).

The used sub-models, which are blocks of different dimensions, can also be represented as:

\[ m_i = \{ I, P, f_i, x_i, y_i, \Omega \} \]

Then the components of the original model are described through the components of elementary models as follows:

\[ \mathbf{M} = \{ m_i \}, \Phi = \{ f_i \}, i \in [1, N_m] \]

\[ (\forall x) P(X) \Leftrightarrow \left[ P_1(X_1) \wedge P_2(X_2) \wedge \ldots \wedge P_{N_m}(X_{N_m}) \right] \]

\[ X = \bigcup_{i=1}^{N_m} X_i; \quad Y = \left( \bigcup_{i=1}^{N_m} Y_i \right) / X \]

\[ Z = \bigcup_{i=1}^{N_m} Z_i; \quad \Omega = P_z Z_i(\Omega); i = 1, 2, \ldots, N_m \]

\[ P_z Z_i(\Omega) \] is the projection of the set onto the hyperplane, the coordinates of which are the components of the vector \( Z_i \).

Such forms of representation of computational models allow generalizing the procedures associated with the formation of modeling algorithms and presenting them as formal problems solved on the basis of these models.

Let us consider the creation of a technological modeling system using the example of the process of dehydrogenation of n-paraffins.

The mathematical model of the dehydrogenation process of higher n-paraffins is a system of differential equations:

\[ G \frac{\partial c_i}{\partial z} + G \frac{\partial c_j}{\partial y} = (1 - \varepsilon) \sum_{j=1}^{N} \eta_j, \quad i = 1, \ldots, M, j = 1, \ldots, N \]

where \( G \) is the consumption of raw materials, \( m^3/\text{h}; C_j \) - concentration of the \( j \)-th hydrocarbon, \( \text{mol/m}^3 \); \( V \) - volume of the catalyst, \( m^3 \); \( \varepsilon \) - porosity of the catalyst layer, \( \varepsilon = 0 \ldots 1; \eta_j \text{-rate of the } j \text{-th reaction, mol/m}^3 \text{h}; \)
The heat balance equation in differential form is written as:

\[ G \frac{\partial T}{\partial z} + G \frac{\partial T}{\partial V} = -(1 - \varepsilon) \sum_{j=1}^{N} \left( \Delta H_{j} \right) c_f \]

Where \( T \) is the process temperature, \( K \); \( \Delta H_j \) - heat of reaction, J/mol; \( c_f \) is the heat capacity of the mixture, J/kg · K.

Initial and boundary conditions:

\[ z = 0: C_i = 0, T = T_{1\alpha} \]

Thus, the dimension of the system of equations of the mathematical model suits with the amount of substances, the concentration of which is determined in the calculations, plus one equation for determining the temperature profile over the reactor. It is a table containing the output concentration of fluxes at a certain date of calculation.

On the basis of a simulation experiment in the dehydrogenation reactor carried out using a technological modeling system, a smooth rise in the temperature of the inlet stream from 469 C\(^0\) to 477 C\(^0\) was observed (Figure 1). At the same time, there were small temperature drops due to a change in the load of raw materials. The coke concentration was 1.3 wt%.

![Figure 1](image)
In the modeling system for the synthesis of linear alkylbenzenes, a production-frame model is implemented to determine the causes of emergencies in the apparatus included in the technological scheme of the installation. The model also demonstrates the actions of personnel to eliminate this emergency. The user selects the device where the emergency occurred, then selects the emergency. After choosing a situation, a list of possible causes its occurrence and the procedure for personnel action to eliminate it appear.

One of the most important issues concerning the further support of programs has become the adaptation of modeling systems. For this, a so-called application initialization file is generated. This module is designed to transfer data to programs describing technological processes. The module is designed in such a way that its internal procedures, with a slight change in the sensor initialization file, are able to retrieve data from any production plant.

The main advantage of the CCM is the optimization calculations. So, modeling the process of hydrogenation of diolefins showed that the optimal consumption of the selective poison, dimethyl disulfide, allows it to increase the yield of the target product, linear alkylbenzene, can be increased by 2.0 ... 14.0%, which is approx. 45-315 million sums / year of additional income, practically without increasing costs at other stages of this production.

**Conclusion**

Thus, the developed modeling systems for oil refining and petroleum chemistry are software products that are of great applied value and provide timely monitoring, accurate forecasting and optimization calculations, including those based on economic criteria.

The developed modeling system of alkylbenzene synthesis processes includes a module for diagnosing the causes of deviations in the operation of an industrial plant and can be used to organize the actions of personnel in the event of emergency situations in the apparatus included in the technological scheme of the plant.

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