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Expert Systems Modeling and Design of High Technological Devices

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Abstract. The article suggests the logical block-scheme of the algorithm of decision making while choosing and designing a device for chemical and teachnological system. Using elements of Boolean algebra, trends in realization of module approach to creating highly efficient equipment have been formulated. 'Artificial intelligence', allowing to create methodology of designing highly efficient technological schemes have been formulated as well.

Keywords: Expert system, mathematical model, heterogeneous-catalytic reactor;

1. Introduction

Complication of modern chemical and technological systems (CTS) and their elements stipulate contradictoriness of various requirements, specified to the equipment, that is chemical and technological devices (CTD). For instance, requirements of efficiency improving and providing wide rangeof sustainable work come into conflict with requirements of decreasing power- and material intensity of the equipment. The other typical sample is contradiction between tendencies of inventors and engineer-technologists to original, non-traditional engineering desicion and aspiration of mechanical engineers to standartization and unification of the equipment. The one of ways of overcoming such contradictions is to create non-traditional devices from traditional unified part (modules) to implement the most important (limiting) technological operations and employing standard CTD at auxiliary (non-limiting) stages of the technological process.

While designing CTD or creating CTS 3 basicallydifferent situations [1] arise:

1) the desicion on employing standard technological device from the catalogue of standard equipment, branch normals and etc. is made;
2) the desicion on necessity of creating non-traditional technological device is made, meanwhile the realization of this desicion relies on combiningthe simplest unified standard constructive elements (modules), produced by industry and lined in unified parametrical range with various standard dimensions, that is the question is not about choice of standard device in whole, but about its construction (assembly) from standard constructive elements (modules);
3) the desicion on necessity of creating non-traditional technological equipment based on creative searching design, desicion of inventive tasks employing new physical principles of operation are made.

The logical block-scheme of the algorithm of decision making when choosing and designing the device for CTS taking into consideration three specified situations is shown in Pic.1.

To formalize the given strategy of decision making while designing technological devicesthe mathematical device of constructing (Boolean) model of device construction [2] is considerably adequate. According to this approach the construction of technological device is given in total of standard functionally constructional elements. Functionally constructional element has a meaning of distinguishing feature and can correspond both to concrete physical characteristics, for instance, surface of heat exchange in the reactor, and to qualitative characteristics or properties, for instance stationary or movable layer of the catalyzer, direction of heat carrier motion and so on. Presence or absence of functionally constructional element correspond to the inclusion or exclusion of the certain member in the system of logically algebraic equations or changing functional form of equations, making mathematical description of device designing. The functionally constructional element Z_i is accepted, has been included into the given construction, if $Z_i = 1$; record $Z_i = 0$ means, that it is absent in the given construction.

Then the formal record of the device construction in the form of logically algebraic (Boolean) model will expressed as:

$$\varphi(Z_1) = \mathop{\Lambda}_{k=0}^{m} \left(\mathop{V}_{k=0}^{m} Z_i \right)_k$$

where Z_i - Boolean variables, connected by logical symbols of totality V and crossing Λ.

At present three trends in realization of module approach to creating highly efficient equipment [3] has clearly been defined.

1. The first trend relies on release of substances group, similar in physico-chemical properties, as well as in technological and built-in implementation of their production. Then for each group of unified devices built-in and technological complex, intended for producing concrete set of chemical products is created. The received complex as a result has a rigid non- transformable structure. The main difficulty in its employment consists in necessity of cleaning all devices, communications and other systems while changing nomenclature.
2. The second trend consists in development of the united multifunctional non-transformable module block with maximum functional excessiveness, providing the importance of carrying out various chains of technological operations in the same block.
3. The third trend is based on creating easily transformable installations of minimum functional excessiveness from unified technological modules and devices. The realization of installations with easily transformable structure from module blocks in definite measure overcomes the above-mentioned contradiction between tendencies to originality observed by inventors and engineers-technologists considering the specificity of processes and aspiration of mechanical engineers to maximum standardization and unification of the technological equipment.

The decision of the task of creative searching design of the complex technological equipment includes the chain 1-4-5-6-7-14-15-16-17-12-13 in logical block-scheme of the Pic. 1. The realization of these stages within the framework of scientifically engineering trend 'artificial intelligence' is implemented by various methods, among which the most efficient are:

1) morphological analysis and synthesis of technological systems;
2) searching design based on systematized collection;
3) methods of searching physical principles of operation based on data base by physical effects;
4) construction of new technological decisions based on prototypes and others.

Among the mentioned methods the method of morphological case, suggested by Austrian scientist F. Tsviki is the most perspective [2]. Using in complex the fruitful idea of analysis of physical impact of searching design, morphological method and the common strategy of system approach to analysis and synthesis of chemical and technological processes, one can construct efficient methodology of creating highly efficient technological systems, being one of the main aims of our work.

Intensification of production is before everything else provided by creating corresponding highly efficient technological equipment, beginning with individual built-in process units and ending with chemical technological aggregates, complexes and systems [3].

Mathematical statement of the problem of creating both individual chemical technological device (CTD) and chemical technological system (CTS) is in whole common to them and consists in stating a problem of multicriteria optimization with the given set of target functions $\vec{W}$, determining requirements for a designer to being created object, and a constraint vector of two types: restriction of equality type $\vec{F}(\vec{Z})=0$, corresponding to the full mathematical model of being constructed object, and restrictions of inequality type $\vec{Z}_{\min} \le \vec{Z} \le \vec{Z}_{\max}$, corresponding to the conditions of physical realizability of the object and engineering assignment for its construction:

$$\vec{W}(\vec{Z}) = \vec{W}(\vec{X}, \vec{Y}, \vec{T}, \vec{K}, \vec{H}, \vec{M}) \to extr, \tag{2}$$

$$\vec{F}(\vec{Z}) = \vec{F}(\vec{X}, \vec{Y}, \vec{T}, \vec{K}, \vec{H}, \vec{M}) = 0, \tag{3}$$

$$\vec{Z}_{\min} \le \vec{Z} \le \vec{Z}_{\max} \tag{4}$$

where $\vec{F} = \vec{F}(f_1, f_2, ...f_n)$ - vector-function of functional operator of the object, that is, system of equations of its mathematical model; $\vec{Z}$ – vector of varying variable, restricted from above and below on the basis of conditions of physical, technological and constructible realizability of the technological system and engineering assignment; $\vec{T}$ – a vector of the operator of technological effect on the processed medium; $\vec{K}$ – a vector of constructible parameters of the object; $\vec{H}$ – a vector of restrictions for the construction; $\vec{M}$ – a vector of engineering assignment requirements; $\vec{X}$ – a vector of parameters of input flows, coming into technological device or system; $\vec{X}$ – a vector of parameters of output flows – derived products.

Mathematical model of the designed object $\vec{F}(\vec{Z}) = 0$ is the most important constituent of mathematical setting of the problem. It is essential that its structure for individual CTD will be one, and for all CTS – another one [4].

The structure of mathematical model for individual CTD: material-energetic flows come into CTD entry, which are presented by input vector $\vec{X} = (x_1, x_2, ...x_n)$ with the given physico-chemical properties $(a_i^1, a_i^2, ...a_i^c), i = \overline{1, n}$. CTD output is characterized by output flows vector $\vec{Y} = (y_1, y_2, ...y_m)$ with required physico-chemical properties $(b_j^1, b_j^2, ...b_j^c), j = \overline{1, m}$. The vector $\vec{X}$ of input flows is subject to purposeful physico-chemical changes in the vector $\vec{Y}$, which are formalized as an operator of engineering effect $\vec{T}$. The latter one is convergency (superimposition) of the simplest operators of various physico-chemical nature (mechanical $\vec{T}_M$, heat $\vec{T}_T$, hydrodynamic $\vec{T}_Г$, diffusion $\vec{T}_Д$, phase change $\vec{T}_Ф$, chemical change $\vec{T}_X$ and etc.). Each of the constituents of operators $\vec{T}_i$ requires specific conditions of their realization. So, mechanical effect can be realized as vibration, crosspartition, mixing and etc.; phase change as evaporation, condensation, dissolution, crystallization and etc., heat one – as heating and cooling; chemical one – as a chemical reaction, flowing in homogeneous (liquid, gas) medium, heterogeneous medium (liquid–gas– solid), on the surface of the catalyzer and etc., diffusion one – as molecular or turbulent diffusion and etc.

Transformation $\vec{X} \xrightarrow{T} \vec{Y}$ or $\vec{Y} = \vec{T}(\vec{X})$ is realized in the technological device, constructible properties of which are characterized by the vector $\vec{K}i$ of the equipment $\vec{K} = (\vec{K}i)$. Restrictions $\vec{H}$ are imposed on device functioning, which can have constructible $\vec{H}_k$ and mode $\vec{H}_p$ character, as well as a set of requirements $\vec{M}$ and flexibility ($\vec{M}_Г$), ecological security ($\vec{M}_Э$) and etc.

Hence, mathematical model of the created technological device is of the form of:

$$\vec{Y} = \vec{T}(\vec{X}, \vec{K}, (\vec{K}_o, \vec{K}_в, \vec{H}(\vec{H}_K, \vec{H}_p), \vec{M});$$

$$\begin{gathered} \vec{T} = (\vec{T}_M, \vec{T}_T, \vec{T}_Г, \vec{T}_Д, \vec{T}_X, \vec{T}_Ф); \\ \vec{K} = (\vec{K}_o, \vec{K}_в) = (k_1, k_2, ..., k_a); \\ \vec{H} = (\vec{H}_K, \vec{H}_p) = (h_1, h_2, ..., h_в); \\ \vec{M} = (\vec{M}_Г, \vec{M}_Э) = (m_1, m_2, ..., m_c); \end{gathered} \tag{5}$$

To constitute a mathematical model of CTS, consisting of a set of individual technological devices, that is it represents a certain set of mathematical models of the type (5). At that, inclusion of individual devices by direct and inverse links is being taken into consideration.

The block-scheme (Fig.2) corresponds to the mathematical model (5).

As a mathematical model of built-in-process module, heterogeneous-catalytic reactor of phosphine oxidation developed by us, we will mention generalized mathematical model, describing both stochastic and determinate properties of polydispersephysico-chemical systems [5]:

$$\frac{\partial p(x,y,t)}{\partial t}+\sum_{i=1}^{3}\frac{\partial}{\partial x_i}[V_i(x,t)p(x,y,t)+\frac{\partial}{\partial \tau}[\frac{\partial \tau}{\partial t}p(x,y,t)]+\frac{\partial}{\partial l}[\frac{\partial l}{\partial \tau}p(x,y,t)]+$$
$$+\sum_{k=1}^{n}\frac{\partial}{\partial c_k}[I_k p(x,y,t)]+\frac{\partial}{\partial T}[p(x,y,t)\sum_{j=1}^{n}\frac{\Delta H_j}{C_p}I_j]+\frac{\partial}{\partial \rho}[\frac{\partial \rho}{\partial t}p(x,y,t)]+ \quad (6)$$
$$+\frac{\partial}{\partial \mu}[\frac{\partial \mu}{\partial t}p(x,y,t)]=q[p(x,y,t),t].$$

where: $y=(\tau,l,\tau_1,\tau_1,\tau_2,...,\tau_n,T,\rho,\mu)$; $I_k=\frac{dC_k}{dt}$ – rate of chemical reaction in dispersed phase along k-key component; n – a number of key components, reacting in dispersed phase; ΔH_j – thermal effect of j-reaction; N – a number of reactions in dispersed phase; C_p – volumetric heat capacity of dispersed phase.

The expression $q[p(x,y,t),t]$ is defined by the mechanism of interactions of particles among themselves, as well as by the presence of external sources and runs-off, that is characterizes the rate, appearance and disappearance of new particles at the moment of the time t of particles with coordinates x, y. As internal coordinates such physico-chemical characteristics as particle residence time in the device τ, typical linear size of the particle l, concentration of the key component in the particle C_k, temperature T, density ρ, viscosity μ .have been accepted.

2. Conclusions

Equation of the balance of particles ensemble properties (6) has sufficiently universal character itself. It is an effective means of describing stochastic sides of many chemico-technological processes in polydisperse media, flowing in heterophase systems.

We performed numerical experiments, taking into account the kinetic models of oxidation of phosphine to palladium catalyst, which yielded good results.

In this research, the methodology of choice and design of high-intensity technological equipment with the use of mathematical models of fluid dynamics, heat and mass transfer and kinetics of the process.

3. References

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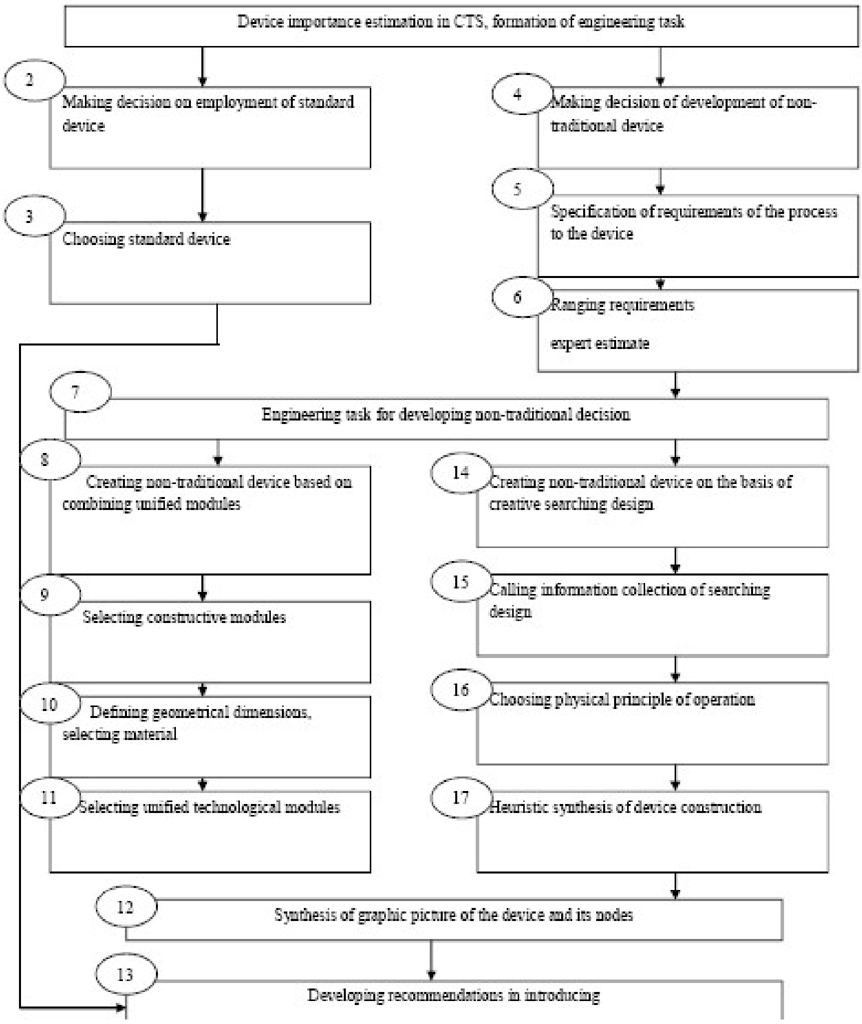

Fig 1. Logical block-scheme of the algorithm of choice and design of the device for CTS

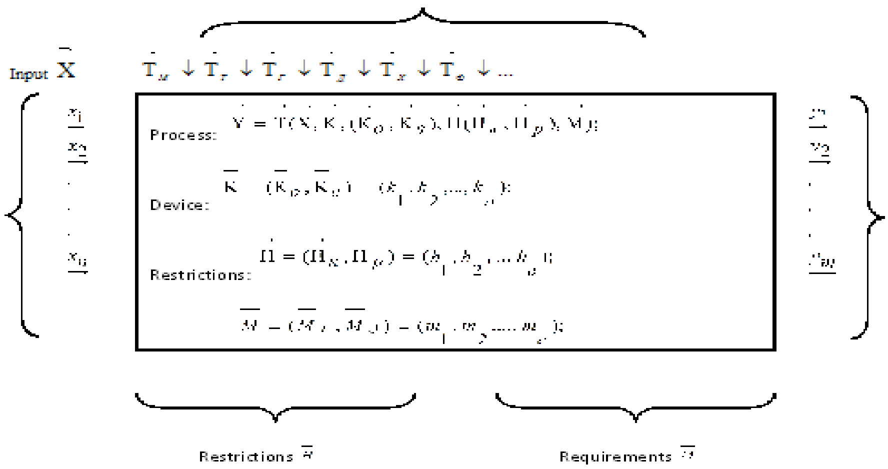

Fig. 2 Block-scheme of the mathematical model (5) of built-in-process module.