# A SYSTEMIC APPROACH TO THE DEVELOPMENT OF COMPUTER-AIDED COMBINED PRODUCTIONS

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UDC 66.01:007.1.005

*A new approach is suggested in designing combined technological systems based on the information theory and thermodynamic principles. The approach allows the solution of particular resource-saving problems as a single problem by increasing the organizational degree of the object.*

One of the ways for creation of resource-saving ecologically clean technological systems is to combine several processes in series or series-parallel units when products, semi-products, or wastes of one production serve as the raw material for another. It occurs most often when the primary processing of solid fossil fuels in semi-products, particularly coal in synthesis gas, is combined with their subsequent processing in the final commercial product, particularly, synthesis gas in hydrogen or ammonia or methanol in benzine. In this case the object of study is a combined processing system with the continuously increasing complexity. Coordination of the local problem of particular processes and subsystems within a combined process and determination of its perspective development is the scientific aspect of creating a computer-aided technological process. When solving the problem, it is necessary, first of all, to establish the research strategy for combined productions.

**Research Strategy**. At present there is no theory for constructing computer-aided production. It may be suggested that the problem will be solved first at the level of particular processes and systems with optimal parameters of their organization sought for from the operation criteria. Then, after the economic problem has been solved, a certain compromise is to be found between the local subsystem optima which is the final solution. This approach can hardly be general, both regarding the research method and the results. Some matters which are the most important at present, particularly, environment protection, are not covered by the approach at all. Consequently, it is necessary to find a universal approach that would give an objective solution to the problem, including the most essential aspects of the production process — ecological and economic — without separating them from each other. To do this, it is necessary to reject solution of particular optimization problems and to look at the objects of study from the point of view of their organization, their generality and specificity, and their potential development, that is, to consider them within the framework of objective laws governing the construction of technological objects. Such an objective law for constructing organized technological systems is formulated in [1]. It was shown that an organized system as an entity had a minimal internal energy level because of the low outside energy inflows and a maximum utilization of internal useful energy resources, including secondary ones, that in an organized technological system is energy-saving. On the other hand, the fact that technological systems tend to self-sufficiency (integrity) as follows from their optimal organization principle is a basis for creating combined productions when products (or wastes) of one are a raw material for another. In addition, organization characteristics of particular units directly responsible for the processing of the raw material depend on the transformation degrees which are increased as the processing organization is increased, the latter increase reduces the waste amount. Minimization of energy and material wastes and combined use of the products (including the wastes) characteristic of organized production systems reflect the ecological aspect of developing combined productions. Moreover, the organization characteristics of production processes include power and nonpower expenditures (process organization expenditures) and in this sense they are closer to economic or, more exactly, thermoeconomic estimates [2].

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D. I. Mendeleev Moscow Technological Institute, Moscow. Translated from Inzhenerno-fizicheskii Zhurnal, Vol. 64, No. 1, pp. 88-98, January, 1993. Original article submitted October 24, 1991.

1062-0125/93/6401-0071$12.50 

Analysis of the factors that influence the technological system organization [1] shows that the characteristics of particular process and subsystem coordination which locate them within the whole structure of power interaction (macrolevel characteristics) are of critical importance whereas the organization parameters of the processes themselves (microlevel characteristics) are secondary. In view of this, the strategy for constructing an organized combined production follows the "top-to-bottom" principle. At the top level local subsystems are coordinated, at the bottom the organization parameters (intensive parameters) of the subsystem components are sought for with account of the obtained information on the extensive subsystem parameters.

**Development of the Coordinating Algorithm.** The coordinating algorithm for constructing a computer-aided combined production consists of three steps: scaling of the thermodynamic properties of the combined process components; decomposition into quasiclosed subsystems (they do not interact energetically); the optimization procedure of selecting coordinated subsystem parameters (see Fig. 1). Scaling and estimation of average energy levels of the processing conversions, as well as plotting of the average energy levels and decomposition into energetically noninteracting subsystems, are given in [3] and the calculation procedure for the energy fluctuation probability may be found in [4]. Therefore in this article we will dwell on the optimization procedure for selecting the extensive datum parameters of the subsystems.

In this case the initial information may be presented as follows:

$$\sum_{i=1}^{I} n_{mi} \langle U_{mi} \rangle = \langle U_m \rangle = \overline{U}_m, \tag{1}$$

where $i = \overline{1, I}$ is the number of elements (according to the number of conversions in the m-th subsystem);

$$\sum_{i=1}^{I} n_{mi} = 1; \tag{2}$$

$$\sum_{m=1}^{M} n_m = 1, \tag{3}$$

where M is the number of quasiclosed subsystems

$$\sum_{m} n_m \langle U_m \rangle = \langle U_e \rangle . \tag{4}$$

The set of equations (1) characterizes the generalized internal energy fluctuations in the subsystems that coincide with the subsystem integrity indicators (average characteristics of a closed subsystem).

Equations (2) and (3) are the normalization conditions for fluctuation probabilities (weight factors) of the internal energies of the subsystem elements and the whole subsystems. The mathematical expectation of the internal energy of the system reflecting the combined process is calculated from relation (4). In accordance with the technological system organization principle at the upper hierarchical levels, macroentropy is a system organization characteristic

$$H_M = -\sum_{m} n_m \ln n_m, \tag{5}$$

whose maximum indicates the highest organization of the system. In order to find the function maximum from (5) with constraints of the type of the equalities (3) and (4), use will be made of the undetermined Lagrangian method. The Lagrangian expression will be of the form

$$L_M = -\sum_{m} n_m \ln n_m - (\lambda_0 - 1)\left(\sum_{m} n_m - 1\right) - \beta\left(\sum_{m} n_m \langle U_m \rangle - \langle U_e \rangle\right). \tag{6}$$

The system of the necessary extremum conditions $L_M$, $\partial L_M/\partial n_m = 0$ (m = 1, 2, ..., M), with statistical independence of the generalized energy fluctuation probabilities included, leads to calculation of the optimal probabilities

$$n_m^{opt} = \exp(-\lambda_0 - \beta \overline{U}_m). \tag{7}$$

The constant factor $\lambda_0$ is found from the normalization condition (3)

$$\sum_{m} \exp(-\lambda_0 - \beta \overline{U}_m) = 1, \tag{8}$$

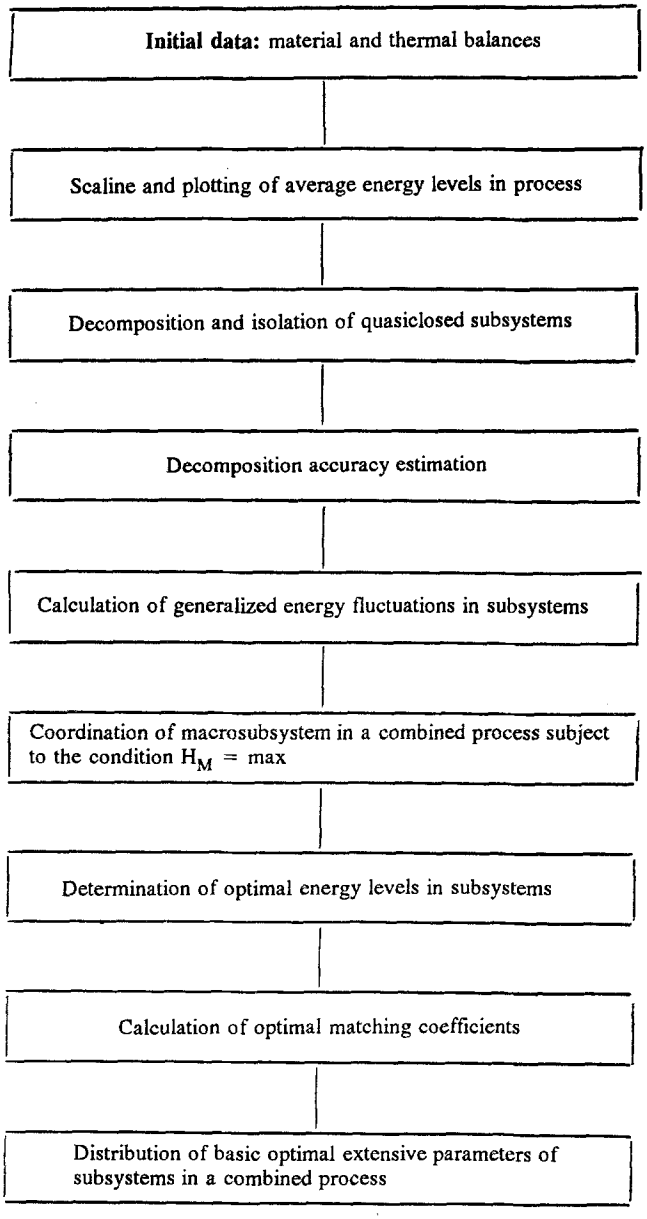


Fig. 1. Block diagram of the coordinating algorithm.

hence

$$\lambda_0 = \ln\left(\sum_m \exp\left(-\beta \bar{U}_m\right)\right). \tag{9}$$

Bearing in mind that $\beta = 1/RT_e$ ($RT_e$ is the energy level of the system representing the combined process), we arrive at:

$$n_m^{opt} = \frac{\exp\left(-\dfrac{\bar{U}_m}{RT_e}\right)}{\sum\limits_m \exp\left(-\dfrac{\bar{U}_m}{RT_e}\right)}, \quad m = 1, 2, \ldots, M. \tag{10}$$

The optimal values of the generalized energy fluctuation probabilities in the subsystems are related to the optimal values of their energy levels by

$$\bar{U}_m^{opt} = RT_e \ln \frac{1}{n_m^{opt}}, \quad m = 1, 2, \ldots, M. \tag{11}$$

Using the notation $\bar{U}^{opt}_m/\bar{U}_m = \varepsilon^{opt}_m$, we obtain the matching correction factors for calculating extensive parameters for each subsystem (m = 1, 2, ..., M). Then, the expression for the generalized energy fluctuations in the subsystems will become

$$\bar{U}^{opt}_m = \bar{U}_m \varepsilon^{opt}_m = \sqrt{\frac{\sum_{i=1}^{I} \bar{C}^2_{Vmi} (\varepsilon^{opt^2}_m \Delta T^2_{smi})}{I}}. \tag{12}$$

Consequently, extensive parameters proper (molar flow rate ratios) will be calculated as

$$\varepsilon^{p}_{mi} = \varepsilon_{mi} \varepsilon^{opt}_m, \tag{13}$$

where $\varepsilon_{mi}{}^{p}$ is the real (corresponding to the optimal organization conditions) mole fraction of the i-th flow in the m-th subsystem; $\varepsilon_{mi}$ is the initial mole fraction (chosen as the first approximation) of the i-th flow in the m-th subsystem; $\varepsilon^{opt}{}_{m}$ is the optimal matching coefficient of the m-th subsystem.

The values of $\varepsilon_{mi}{}^{p}$ for the subsystem elements determine the extensive flow parameters in the combined process which are assumed to be preset and constant in solving the problem at the lower hierarchial level, i.e., determining the parameters of optimal organization of the subsystem components.

**The Algorithm for Determining the Optimal Subsystem Organization Parameters.** In accordance with the informational (systemic) approach the efficiency function of a chemical engineering system is defined by

$$F(\bar{x}_n) = 1 - \eta_c, \tag{14}$$

where

$$\eta_c = \frac{\sum_{i=1}^{I} n_i I_{0i} \eta_i}{\sum_{i=1}^{I} n_i I_{0i}}. \tag{15}$$

Here $n_i$ is the weight factor characterizing the mean thermodynamic level location of the i-th process $\bar{U}_i$ relative to the whole system level of $RT_e$. The weight factors satisfy the normalization condition and are defined by an expression of the form $n_i = \exp(-\bar{\Delta U}_i/RT_e)$, $I_{0i}$ is the maximum amount of information of the i-th conversion (the reversible process information amount). As is known, the ordering measure characteristic $I_{0i}$ is related to the entropy change $\Delta H_i$ by Shennon–Wiener's equation

$$I_{0i} + \Delta H_i = 0.$$

In equality (15) the information efficiency value is denoted by $\eta_i = I_{ir.i}/I_{0i}$, where $I_{ir.i} = I_{0i} - \Delta I_{ir.i}$ is the real information amount of the i-th conversion which includes real thermodynamic process irreversibility following from the second thermodynamic law. The efficiency of the system consisting of I additive processes and, consequently, the efficiency function F depend on n optimizable parameters $x_1, x_2, \ldots, x_n$.

At the first stage of the optimization problem solution the search procedure for optimal mean energy levels of every i-th process in the system considered at known $I_{0i}$ and $I_{ir.i}$ (the short-range forecast problem) is of interest. It should be also noted that a technological system (at a hierarchial level considered) is meant as a quasiclosed system isolated in a specific way.

For determination (at fixed $I_{0i}$ and $I_{ir.i}$) of the optimal weight factors $n^{opt}{}_{i}$ characterizing the mean thermodynamic levels, the derivative $\partial\eta_c/\partial n_i$ will be found from (15). For the necessary conditions of extremum existence with the statistical independence of $n_i$ being taken into consideration, we obtain after some transformations

$$n^{opt}_i = \frac{1}{I_{0i}|\eta_i - \eta_c|} \Big/ \sum_{i=1}^{I} \frac{1}{I_{0i}|\eta_i - \eta_c|}. \tag{16}$$

On the other hand, since

$$n^{opt}_i = \exp\left(-\frac{c_{Vi}}{2R} \frac{\Delta T^{opt2}_{ei}}{T^2_{ec}}\right), \tag{17}$$

where $c_{Vi}$ is the specific heat of the i-th flow (at V = const), R is the universal gas constant, $T_{ec}$ is the equivalent temperature level of the whole system, then the mean optimum energy level of the i-th process is defined by

$$\Delta T_{ei}^{opt} = \sqrt{\frac{2R}{c_{Vi}} T_{ec}^2 \ln \frac{1}{n_i^{opt}}}. \tag{18}$$

Thus, Eqs. (16) and (18) give the optimal functioning conditions (the input and output parameters) for each element of the technological system considered at a certain mean optimal energy level ($RT^{opt}_{ei}$ = idem). For heat transfer processes the mean optimum energy levels are related to the input and output flow parameters in the element. The input and output gas dynamic process parameters can be determined from the iterative problem solution. For determination of the process flow parameters in the chemical and mass transfer processes, optimization is performed for the microentropy criterion with the condition $H_\mu$ = max.

According to expressions (14) and (15), the organization optimization problem proper assumes $n_i$, $I_{0i}$, and $I_{ir.i}$ to be estimated as functions of thermal, gas dynamic, mass transfer, and chemical process parameters for every i-th component of the system. The energy subsystem elements directly responsible for processing useful energy of different forms and potentials are the most essential in the organization of technological systems.

We will find the desired quantities in expression (15) for the most typical elements of energy subsystems in chemical engineering. As follows from [5], in the case of polytropic compression of gases (vapors) the following expressions hold

$$I_{0i} = (1 + \delta_{ad}) \frac{T_{in\,i}}{T_{av\,i}\eta_{ad}} \left(\frac{p_{out\,i}}{p_{in\,i}}\right)^{(1+\delta_{ad})\frac{T_{in\,i}}{T_{av\,i}\eta_{ad}}} \ln \frac{p_{out\,i}}{p_{in\,i}},$$

$$\eta_i = \eta_{ad} \left(\frac{p_{in\,i}}{p_{out\,i}}\right)^{(1+\delta_{ad})\frac{T_{in\,i}}{T_{avi}}\left(\frac{1}{\eta_{ad}} - 1\right)}, \tag{19}$$

$$n_i = \exp\left(-\frac{\bar{c}_{Vi}}{2R}\frac{\Delta T_{ei}^2}{T_{ec}^2}\right); \quad \Delta T_{ei} = \varepsilon_i T_{avi}\left(1 + \frac{R}{\bar{c}_{pi}} \ln \frac{p_{out\,i}}{p_{in\,i}}\right).$$

Here $(1 + \delta_{ad}) = A_{ad}/A_i$, and the adiabatic and isothermic work are equal, respectively, to

$$A_{ad} = \frac{k}{k-1} RT_{in\,i}\left[\left(\frac{p_{out\,i}}{p_{in\,i}}\right)^{\frac{k-1}{k}} - 1\right]; \quad A_i = RT_{in\,i} \ln \frac{p_{out\,i}}{p_{in\,i}},$$

where k is the adiabat index equal to the ratio of specific heats at constant pressure and volume: $k = \bar{c}_{pi}/\bar{c}_{Vi}$; $p_{in\,i}$, $p_{out\,i}$ are the input and output pressures in the compressor; $T_{av}$ is the integral mean temperature; $\eta_{ad}$ is the adiabatic efficiency of the compressor ($\eta_{ad}$ = 0.5-0.9); $\varepsilon_i$ is the mole fraction of the i-th flow (from the coordinating algorithm calculation results). The output compressor temperature and power are defined by

$$T_{out\,i} = T_{in\,i} + \frac{T_{in\,i}}{\eta_{ad}}\left[\left(\frac{p_{out\,i}}{p_{in\,i}}\right)^{\frac{k-1}{k}} - 1\right],$$

$$N = \bar{c}_{pi} T_{in\,i} G_i \left[\left(\frac{p_{out\,i}}{p_{in\,i}}\right)^{\frac{k-1}{k}} - 1\right] \Big/ 860\eta_{ad}, \tag{20}$$

where $G_i$ is the molar gas (vapor) flow rate, kmole/h.

For a heating transfer process (a positive temperature gradient) of the main ("cold") flow (the countercurrent heat transfer fluid flows) the balance equations are valid

$$G_{ci}\bar{c}_{pci}(T_{out\,ic} - T_{in\,ic}) = G_{hi}\bar{c}_{phi}(T_{inih} - T_{out\,ih}),$$

$$G_{ci}\bar{c}_{pci}(T_{out\,ic} - T_{in\,ic}) = \bar{k}S\theta_{av}, \tag{21}$$

where the subscript c refers to the main (cold) flow and the subscript h, to the hot one; k is the heat transfer coefficient; S is the heat transfer surface area; $\theta_{av}$ is the average motive force of heat transfer. It follows from (21) that

$$T_{\text{out ic}} = \frac{T_{\text{in ic}} G_{\text{ci}} \bar{c}_{p\text{ci}} + \frac{\bar{k}S}{2}\left[2T_{\text{in ih}} - T_{\text{in ic}}\left(1 - \frac{G_{\text{ci}}\bar{c}_{p\text{ci}}}{G_{\text{hi}}\bar{c}_{p\text{hi}}}\right)\right]}{G_{\text{ci}}\bar{c}_{p\text{ci}} + \frac{\bar{k}S}{2}\left[1 + \frac{G_{\text{ci}}\bar{c}_{p\text{ci}}}{G_{\text{hi}}\bar{c}_{p\text{hi}}}\right]},$$

$$T_{\text{out ih}} = T_{\text{in ih}} - \frac{G_{\text{ci}}\bar{c}_{p\text{ci}}}{G_{\text{hi}}\bar{c}_{p\text{hi}}}(T_{\text{out ic}} - T_{\text{in ic}}). \tag{22}$$

In this case the following expression is valid for the information characteristics

$$I_{0i} = \frac{\bar{c}_{p\text{ci}}}{R}\frac{1}{\eta_T}\left(\frac{T_{\text{out ic}}}{T_{\text{in ic}}}\right)^{\frac{\bar{c}_{p\text{ci}}}{R\eta_T}} \ln\left(\frac{T_{\text{out ic}}}{T_{\text{in ic}}}\right),$$

$$\eta_i = \eta_T\left(\frac{T_{\text{in ic}}}{T_{\text{out ic}}}\right)^{\frac{\bar{c}_{p\text{ci}}}{R}\frac{T_{\text{inih}} - T_{\text{out ic}}}{T_{\text{out ic}} - T_{\text{in ic}}}}, \tag{23}$$

$$n_i = \exp\left(-\frac{\bar{c}_{V\text{ci}}}{2R}\frac{\varepsilon_{\text{ci}}^2 T_{\text{av ic}}^2}{T_{\text{ec}}^2}\right).$$

Here the thermodynamic efficiency of the heat exchanger $\eta_T$ is

$$\eta_T = (T_{\text{out ic}} - T_{\text{in ic}})/(T_{\text{in ih}} - T_{\text{in ic}}).$$

Similarly, for a cooling heat exchanger (a negative temperature gradient) which cools the main ("hot") flow, we obtain

$$I_{0i} = \frac{\bar{c}_{p\text{hi}}}{R}\frac{1}{\eta_T}\left(\frac{T_{\text{in ih}}}{T_{\text{out ih}}}\right)^{\frac{\bar{c}_{p\text{hi}}}{R\eta_T}} \ln\frac{T_{\text{in ih}}}{T_{\text{out ih}}},$$

$$\eta_i = \eta_T\left(\frac{T_{\text{out ih}}}{T_{\text{inih}}}\right)^{\frac{\bar{c}_{p\text{hi}}}{R}\frac{T_{\text{out ih}} - T_{\text{in ic}}}{T_{\text{in ih}} - T_{\text{out ih}}}}, \tag{24}$$

$$\eta_T = (T_{\text{in ih}} - T_{\text{out ic}})/(T_{\text{inih}}/T_{\text{out ic}}),$$

$$n_i = \exp\left(-\frac{\bar{c}_{V\text{hi}}}{2R}\frac{\varepsilon_{\text{ih}}^2 T_{\text{av ih}}^2}{T_{\text{ec}}^2}\right).$$

In this case from equations similar to (21), it is easy to obtain expressions for $T_{\text{out ic}}$, $T_{\text{out ih}}$ which coincide with (22) correctly within substitution of the subscript h for c and vice versa in both sides of the equality. It should be also noted that for practical calculation of the average heat capacity $\bar{c}_{pi}$ an approximation of the following form can be efficiently used [6]:

$$\bar{c}_{pi} = \sum_{j=1}^{k} N_j\{A_j T_{\text{avj}}^3 + B_j T_{\text{avj}}^2 + C_j T_{\text{avj}} + D_j\}, \tag{25}$$

where k is the number of components in the i-th mixture; $N_j$ is the specific fraction of the j-th component in the mixture; $A_j$, $B_j$, $C_j$, $D_j$ are numbers to be experimentally determined in the temperature range of interest.

The phase transition heat exchangers are the most complicated type. In this case (a two-stage process) expressions (23) and (24) are valid for the information characteristics, and the balance equations, in particular, for cooling, will become

$$G_{\text{hi}}\bar{c}_{p\text{hi}}(T_{\text{pr 1i}} - T_{\text{out ih}}) = G_{\text{ci}} r_{\text{vi}}, \quad G_{\text{ci}} r_{\text{vi}} = (\bar{k}S)_1 \frac{1}{2}[T_{\text{pr1i}} - 2T_{\text{in ic}} + T_{\text{out ih}}],$$

$$G_{\text{hi}}\bar{c}_{p\text{hi}}(T_{\text{in ih}} - T_{\text{pr 1i}}) = G_{\text{ci}}\bar{c}_{p\text{ci}}(T_{\text{out ic}} - T_{\text{in ic}}), \tag{26}$$

$$G_{\text{hi}}\bar{c}_{p\text{hi}}(T_{\text{in ih}} - T_{\text{pr 1i}}) = (\bar{k}S)_2 \frac{1}{2}[T_{\text{in ic}} - T_{\text{out ic}} + T_{\text{pr 1i}} - T_{\text{in ic}}],$$

where $G_{ci} = G_{vi}$; $T_{in\ ic} = T_{bi}$; $r_{vi}$ is the heat of vaporization of the i-th flow. It easily follows from the set (26) that

$$T_{out\ ih} = T_{in\ ih} - \frac{G_{ci} r_{vi}}{G_{hi} \bar{c}_{pci}} - \frac{G_{ci} \bar{c}_{pci}}{G_{hi} \bar{c}_{phi}} (T_{out\ ic} - T_{in\ ic}), \tag{27}$$

and

$$(\bar{k}S)_1 = \frac{2G_{ci} r_{vi}}{2T_{out\ ih} - 2T_{in\ ic} + (G_{ci} r_{vi})/(G_{hi} \bar{c}_{phi})},$$

$$(\bar{k}S)_2 = \frac{2G_{ci} \bar{c}_{pci} (T_{out\ ic} - T_{in\ ic})}{2T_{in\ ih} - T_{in\ ih} - T_{out\ ic} - [(G_{ci} \bar{c}_{pci})/(G_{hi} \bar{c}_{phi})](T_{out\ ic} - T_{in\ ic})}, \tag{28}$$

$T_{out\ ic}$ is a fixed value. It is noteworthy that if in (26) $\bar{c}_{pci} = 0$ is assumed, the set (26) will be identical to (21) valid for a hot (main) flow.

In a more general case (a three-stage process) we have

$$\begin{gathered}
G_{hi} \bar{c}_{phi} (T_{in\ ih} - T_{pr\ 1i}) = G_{ci} \bar{c}_{pci} (T_{out\ ih} - T_{in\ ic1}), \\
G_{hi} \bar{c}_{phi} (T_{in\ ih} - T_{pr\ 1i}) = (\bar{k}S)_1 \frac{1}{2} [T_{in\ ih} - T_{out\ ic} + T_{pr1i} - T_{in\ ic1}], \\
G_{hi} \bar{c}_{phi} (T_{pr1i} - T_{pr\ 2i}) = G_{ci} r_{vi}, \\
G_{ci} r_{vi} = (\bar{k}S)_2 \frac{1}{2} [T_{in\ ic1} - 2T_{in\ ic1} + T_{pr\ 2i}], \\
G_{hi} \bar{c}_{phi} (T_{pr\ 2i} - T_{out\ ih}) = G_{ci} \bar{c}_{pci} (T_{in\ ic1} - T_{in\ ic2}), \\
G_{hi} \bar{c}_{phi} (T_{pr\ 2i} - T_{out\ ih}) = (\bar{k}S)_3 \frac{1}{2} [T_{pr\ 2i} - T_{in\ ic1} + T_{out\ ih} - T_{in\ ic2}].
\end{gathered} \tag{29}$$

Consequently,

$$T_{out\ ih} = T_{in\ ih} - \frac{G_{ci}}{G_{hi} \bar{c}_{phi}} [\bar{c}_{pxi} T_{out\ ic} + (\Delta c_{pci} T_{in\ ic1}) - c_{pci} T_{in\ ic2}] - \frac{G_{ci} r_{vi}}{G_{hi} \bar{c}_{phi}},$$

$$(\bar{k}S)_1 = \frac{2G_{ci} \bar{c}_{pci} (T_{out\ ic} - T_{in\ ic1})}{2T_{in\ ih} - T_{out\ ic} \left(1 + \frac{G_{ci} \bar{c}_{pci}}{G_{hi} \bar{c}_{phi}}\right) + T_{in\ ic1} \left(\frac{G_{ci} \bar{c}_{pci}}{G_{hi} \bar{c}_{phi}} - 1\right)},$$

$$(\bar{k}S)_2 = \{2G_{ci} r_{ci}\} \left\{ T_{in\ ih} + T_{out\ ih} - 2T_{in\ ic1} + \frac{G_{ci}}{G_{hi} \bar{c}_{phi}} [(\bar{c}_{pci1} + \bar{c}_{pci2}) T_{in\ ic1} - \bar{c}_{pci1} T_{in\ ic2} - \bar{c}_{pci2} T_{out\ ic}] \right\}^{-1}, \tag{30}$$

$$(\bar{k}S)_3 = \frac{2 \bar{c}_{pci1} G_{ci} (T_{in\ ic1} - T_{in\ ic2})}{2T_{out\ ih} - T_{in\ ic1} \left(1 - \frac{\bar{c}_{pci1} G_{ci}}{G_{hi} \bar{c}_{phi}}\right) - T_{in\ ic2} \left(1 + \frac{\bar{c}_{pci1} G_{ci}}{G_{hi} \bar{c}_{phi}}\right)}.$$

The calculation procedures given here are used in the general algorithm of solving the problem for every subsystem. The algorithm for calculation of the optimal intensive parameters for the subsystems is shown in Fig. 2.

1. Assignment of the initial data to be input: the element number in the subsystem considered, sequences of the standard elements in the subsystem considered in accordance with their location in the subprogram library, the number of heat exchangers, compressors, the total number of optimizing parameters in the system, vector of the initial optimizing parameter values (in their succession in the system). The quantities characterizing the required computation accuracy: the maximum allowable number of steps and the minimal admissible step $\varepsilon^*$.

2. Forming the optimizing arrays and providing the cycle for variables (k) to be varied.

3. Computation of the efficiency function F (14), account of positivity of the quantities characterizing the system elements considered.

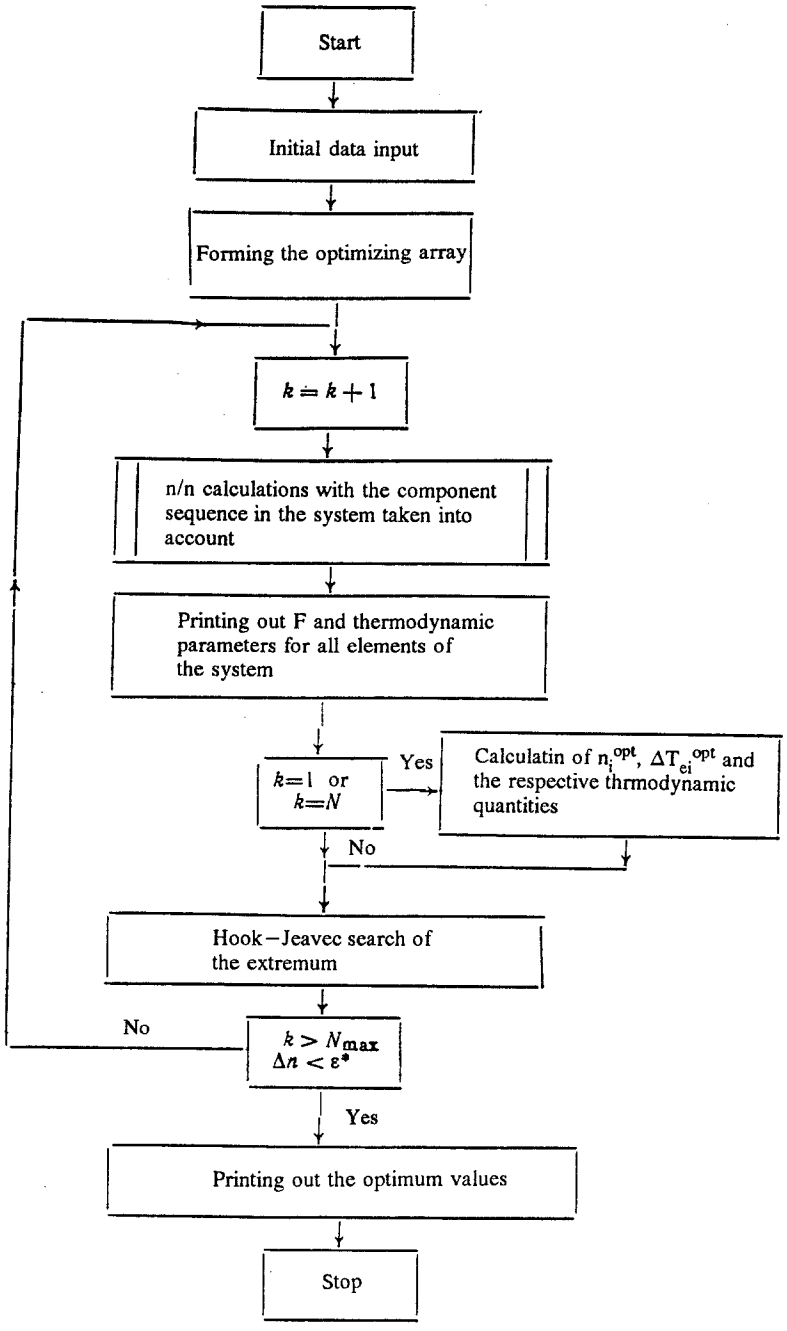


Fig. 2. Computation algorithm for optimum parameters of the subsystem organization (simplified block diagram).

4. Printing out the F function, indicating the step number and all the necessary parameters of every element of the subsystem (19)-(30).

5. For k = 1 (and at the last computation step) computation of $n^{opt}_i$ and $\Delta T^{opt}_{ei}$ from (16) and (18) and iterative solution of the equations for the respective thermodynamic quantities with expression (19) taken into consideration.

6. Optimization (search of the efficiency function extremum) by Hook-Jeavce method.

7. Checking of the computation stop conditions ($k > N_{max}$; $\Delta n < \varepsilon^*$).

8. Printing out the optimal values, including F, $\Delta n$, and N (the number of optimization steps).

The above algorithm was realized on a Solar 16-65 MATRA computer in the RTES-D system. The program language was FORTRAN.

The systematic approach suggested was used as a basis for development of a computer-aided combined process of coal gasification and alcohol production. Realization of the coordinating algorithm gave consumption indices providing an

integral relation of coal expenditure per 1 ton of methanol and a higher alcohol mixture of −1.388. The optimum output of the final stage (alcohol production) is slightly above 300,000 tons of mixture per year. Prognosis of the intensive parameter development (the lower unit optimization results) will drastically change the initial range of products at the production, reducing it to methanol alone. At the present optimization stage intensive parameters of the subsystem elements are determined. They may be used to outline the ways of varying the power and process parameters in order to select the optimal element structure of a combined production. In particular, pressure in the section for synthesis gas separation from sulfuric compound and carbon dioxide was predicted to change from 5.5 to 7.0 MPa, thus increasing the degree of harmful impurity separation, decreasing emissions, and increasing the output of the commercial product, sulfur, produced from washed sulfuric compounds.

## CONCLUSIONS

1. The suggested systemic approach to the development of computer-aided combined productions is realized following the general research strategy from the general to the particular, from coordination of the local problems for separate macroscopic quasiclosed subsystems to determination of optimal organization parameters for individual elements of the subsystems.

2. Because in constructing the organized technological structures their basic laws are used, it is possible to combine effectively the economic and ecological criteria of technological transformations.

3. The principle suggested allows prognosing intensive development of combined productions.

4. Algorithmic and program realization of the approach suggested has a methodical community and can be used in CAD systems at higher levels of combined production.

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