# EQUATION-ORIENTED SIMULATION OF TECHNOLOGICAL SYSTEMS

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The paper presents general notions and methods of the equation-oriented simulation of complex technological systems and introduces a computer-coded simulator of this type.

The simulation of complex systems of chemical technology in steady state became a commonly accepted tool for their analysis and synthesis. To avoid possible misunderstanding, it is necessary to state here that under simulation of a complex technological system the solution of its mathematical model with respect to all corresponding problems is to be understood. By the expression "solution of a mathematical model" one simply means that all the relations and equations representing the bonds and connections among individual elements of the system must be adequately respected and fulfilled for all reasonable values of their variables[1]. Obviously, the level of difficulty of the solution is quite proportional to the number of elements, the non-linearity degree of relations among them and the number of recycle streams in the system. Regardless of possible and known difficulties an immense growth in the development of various simulation methods and algorithm can be observed in the literature of last years. The reason for this progress lies in the introduction of efficient digital computers and the formalization of computation on the basis of standardized flowsheeting.

The presented simulation principles and methods can be subdivided into three main groups: *1*) topology-oriented method which solves any particular mathematical model only in the frame of given elements, the calculations consider and follow the position of any element in the structure of the simulated system, *2*) simultaneous method which obtains all approximations of the seeked solution through the local linearization of the system model as a whole, *3*) equation-oriented method which collects all particular sets of equations, describing the models of individual elements, into the system one and solves it in an especially defined sequence.

## THEORETICAL

The main goal of the development of new calculation principles is to remove all the difficulties connected with the stiff notion of an element in topology-oriented simulation methods and thus to enhance the flexibility of corresponding program systems.

Various claims and approaches how to improve the efficiency of simulation algorithms have been proposed recently, *e.g.*

- to enable numerical inversion of technological streams[2],
- to break up the boundaries of the elements inside the simulated technological system,
- to use simultaneous-modular methods for calculations of technological systems[3,4],
- to develop new simulators on the basis of solution of larger sets of non-linear equations[5],
- to transform the existed topology-oriented simulators into the equation-oriented ones[5],
- to combine topology-oriented and equation-oriented simulation principles[6] *etc.*

The centre of gravity of the problem is at the same time shifted to the comprehensive analysis of the simulated system. Now the starting point for the analysis is not formed by individual elements of the system but by the ordered collection of its mathematical models. And because these models are in principle sets of algebraic equations the simulation approach is named "equation-oriented".

The equation-oriented principle starts from the original structure of the system set of equations and relations describing the technological system under question. It seeks further especial features of the set (structural and analytical art) to utilize them for the most convenient way of solution. It is necessary to algoritmize four basic steps for this purpose: *1*) determination of an output variable for any equation of the set, *2*) separation of solvable subsets, *3*) determination of an "optimal" sequence of solution of individual equations and subsets, *4*) solution of individual subsets as the solution of the simulated system as a whole.

The fundamentals for further development of corresponding computational methods are formed by the works of Steward[7], Himmelblau[8], Ledet and Himmelblau[9], Westerberg and Edie[10], Ramirez and Vestal[11], Soylemez and Seider[12], Stadtherr and Wood[13], Shacham[14] and others. The main goal of determination of output variables vector is to transform the implicit form of equations

$$F_i(x_1, \ldots, x_P, b_1, \ldots, b_A) = 0\,, \quad i = 1, \ldots, B\,, \tag{1}$$

where $x_i$ is set of unknown quantities, $b_i$ set of known quantities, $P$ number of unknown quantities, $B$ number of equations, and $A$ number of known quantities, into an explicit one. There are several possibilities how to do it, as may be illustrated by the following example. Let us have a hypothetic set of equations

$$\begin{aligned} f_1(x_1, x_2) &= 0 \qquad f_2(x_0, x_2, x_3, x_6) = 0 \\ f_3(x_3, x_5) &= 0 \qquad f_4(x_3, x_4) = 0 \\ f_5(x_1, x_4, x_5) &= 0 \quad f_6(x_1, x_6) = 0\,. \end{aligned} \tag{2}$$

There exist fourteen different output variables vectors (Table I), each vector corresponds to different solvable subset with different level of iterative calculation. It is therefore possible to state the following rules: *1*) The selection of output variables vector necessary influences the course of solution as for the extent of iterative calculation. *2*) Proper selection of optimization (control) variables ($P < B$) can give in the best case the straightforward solution schema (*i.e.* the solution without iterations). Consequently, instead of arbitrary selection of an output variables vector, it is necessary to base the selection on a proper algorithm (*e.g.* Ramirez and Vestal[11]). Such an algorithm leads to the determination of "optimal" or "suboptimal" vector of output variables. The simplified RAMIREZ–VESTAL algorithm seeks for an equation to coordinate it with variables, as many as possible, and thus to obtain a calculation schema without loops[15]. The algorithm analyses the structure of the set of equations but neglects the analytical information. To remove this drawback, an algorithm which determines the vector of output variables on the basis of analytical character of the system has been presented[15]. The basic idea of its functioning is given by the sensitivity of the set of equations on the points of its tearing. Partial derivatives are used as a measure of the sensitivty for they describe approximately the absolute error propagation. The algorithm considers, however, the local sensitivity

TABLE I

Vectors of output variables and corresponding number of iterative variables *I* in relation with control variables *O*

| Variant | Function | | | | | | *O* | *I* |
|---|---|---|---|---|---|---|---|---|
| | $f_1$ | $f_2$ | $f_3$ | $f_4$ | $f_5$ | $f_6$ | | |
| 1 | $x_1$ | $x_2$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | | 2 |
| 2 | $x_1$ | $x_2$ | $x_5$ | $x_3$ | $x_4$ | $x_6$ | | 2 |
| 3 | $x_2$ | $x_3$ | $x_5$ | $x_4$ | $x_1$ | $x_6$ | $x_0$ | 1 |
| 4 | $x_2$ | $x_6$ | $x_3$ | $x_4$ | $x_5$ | $x_1$ | | 2 |
| 5 | $x_2$ | $x_6$ | $x_5$ | $x_3$ | $x_4$ | $x_1$ | | 2 |
| 6 | $x_2$ | $x_0$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | | 1 |
| 7 | $x_2$ | $x_0$ | $x_5$ | $x_3$ | $x_4$ | $x_6$ | $x_1$ | 1 |
| 8 | $x_1$ | $x_0$ | $x_3$ | $x_4$ | $x_5$ | $x_6$ | | 1 |
| 9 | $x_1$ | $x_0$ | $x_5$ | $x_3$ | $x_4$ | $x_6$ | $x_2$ | 1 |
| 10 | $x_2$ | $x_0$ | $x_5$ | $x_4$ | $x_1$ | $x_6$ | $x_3$ | 0 |
| 11 | $x_2$ | $x_0$ | $x_5$ | $x_3$ | $x_1$ | $x_6$ | $x_4$ | 0 |
| 12 | $x_2$ | $x_0$ | $x_3$ | $x_4$ | $x_1$ | $x_6$ | $x_5$ | 0 |
| 13 | $x_2$ | $x_0$ | $x_3$ | $x_4$ | $x_5$ | $x_1$ | | 1 |
| 14 | $x_2$ | $x_0$ | $x_5$ | $x_3$ | $x_4$ | $x_1$ | $x_6$ | 1 |

so that only one equation is always explored for this purpose. Global sensitivity of the entire system is thuse not considered, but Gabrisch[2] took up an idea how to consider the sensitivity during the determination of output variables and constructed an algorithm which enables to obtain a global reference about the sensitivity of the system as a whole.

## RESULTS

The free concept of a system element in the equation-oriented simulation enables us to differentiate all the input, output and control variables only as dependent or independent ones. This concept was also the starting point for the following development of the equation-oriented simulator GOS–84 (Gleichungsorientierte Simulation). The implemented methods

- are independent of the orientation of technological streams,
- do not suppose any "black-box" representation in the mathematical models of the simulated system,
- consider partial and global features of the structure of the solved set of equations,
- enable the simulation problem to be described with the aid of standard unit operation and process models,
- enable the user to include his own programs into the simulator without a special knowledge of its structure and functioning.

The program is able to solve the following task: *1*) Generation of the set of equations describing a system and calculation of estimated values. *2*) Investigation of the adjacencies of the individual equation and determination of the outputs of the equations. *3*) Establishment of a course for solving the set of equations and its connection with the system. *4*) Solution of the given set of equations according to the task. *5*) Output of the results of simulation.

As for the models of elements (macros) and analysis- or solution-programs the system is quite open. This fact gives the user the possibility to call individual programs without the necessity of changes in it. The system is constructed namely as a dynamic layer-structure. Outside of the programs- and macros-library two other datainputs are to be used: they serve for program call and system-description. The program package is presented in Fig. 1.

The system consists essentially of three parts working in a sequence. First of all is the set of equations with respect to the structure of the system generated, it takes then a form which may be treated in the second part. The system involves a mode of generation which makes use of models containing the equations in a form which is highly adapted to the traditional notation used by the chemical engineer. They are available as macros in library. The advantage of macros is that the sequence of order is not fixed, but can be changed as required by the parameters transmitted as operands to the macro order. The system can be established stepwise. The generated orders

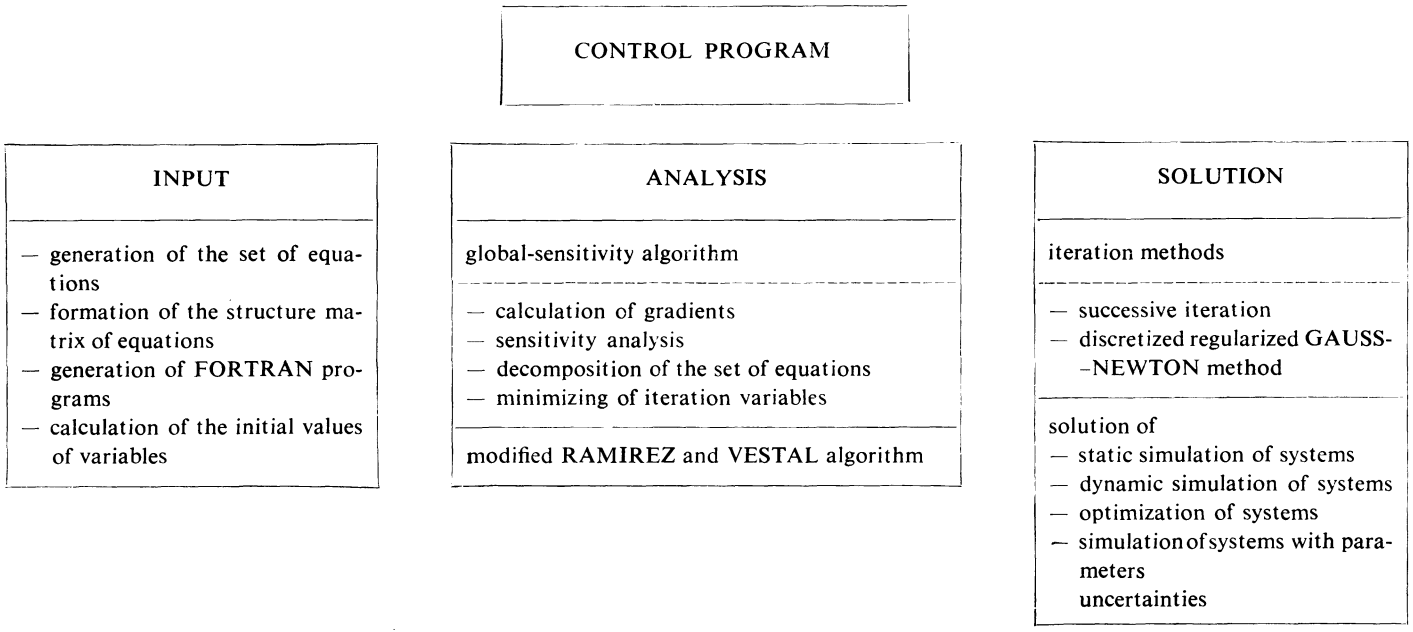


FIG. 1
The structure of the system GOS-84

consist of FORTRAN expressions. Such generations result is a list of equations in analytical form for further treatment. Each dependent variable has its starting approximation calculated. The analysis of the set is performed in the second part, it is possible to choose either the global-sensitivity algorithm[2] or the modified RAMIREZ–VESTAL algorithm[15]. The fundamental idea of the investigation on the basis of global-sensitivities is to rearrange the framework established from the equations and variables describing the system and thus to determine a sequence of calculation with appropriate output assignment in such a way that the simple insertion procedure used for the solution converges with a high degree of certainty. Decomposition is carried out using an algorithm which follows the STEWARD algorithm[7].

The last part, which is close connected with the second one, serves for the solution itself. For equations having been assigned other output variables after the analysis, the zero points are determined according to NEWTON. As regards the iteration method, the direct substitution method or a discretized regularized GAUSS–NEWTON procedure may be chosen.

According to the given problem, the master program controls the sequence of particular subprograms and determines the claims for computer storage.

## DISCUSSION

The schema is evident from Fig. 2. The purpose is to cool xylene (stream 1) from 315·15 K to 241·15 K, using mother liquor (stream 16). The cooling agent is conducted in counter-current in the main flow direction through the jacket, where its temperature rises from 221·15 K to about 311·00 K. This is achieved by using seven tubular exchangers of different geometrical dimensions (Table II). The flow rate of xylene is 11·125 kg/s, that of the mother liquor is 9·25 kg/s. Material data are generally calculated as a third degree polynomial. The overall system of xylene, cooling by mother liquor, involves 222 equations which, as a consequence of the calculation of material data, heat transfer coefficient and temperature, are highly nonlinear. The most important results of the solution are summarized in Tables III and IV. This example is used as a reference because of its nonlinearities as well as of the five tearing points required for topology-oriented simulation. For a more convenient representation of the results, eight possible computational variants of the system have been realized. Apart from the comparison of the above-mentioned methods of approach in the simulation of chemical systems, possibilities of improving the establishment of element programs for the systems operating on a topological basis are also discussed in detail, the following computational variants were realized: *1*) Topology-oriented simulation, using element models established on the basis of an approach from chemical engineering point of view. REGULA FALSI was used as an iteration method for the internal iterations within the elements. *2*) Topology-oriented simulation, using element models established on the basis of global sensiti-

vity studies. Successive iteration was used as an iteration method. *3*) This variant is identical with the second variant with the exception of the iteration method used. REGULA FALSI was employed. *4*) Topology-oriented simulation using inverse information flow (Fig. 3). This inverse information flow, which is difficult to realize

TABLE II

Geometrical data of heat exchangers of xylene cooling by mother liquor

| Parameter | Heat exchanger | | |
|---|---|---|---|
| | 1–4 | 5 | 6, 7 |
| Internal diameter of tube (m) | 0·02 | 0·02 | 0·02 |
| External diameter of tube (m) | 0·022 | 0·022 | 0·022 |
| Number of tubes | 376 | 90 | 376 |
| Length of tube (m) | 6 | 6 | 6 |
| Equivalent area ($m^2$) | 0·0288 | 0·0106 | 0·0453 |
| Equivalent diameter (m) | 0·0245 | 0·0138 | 0·0129 |

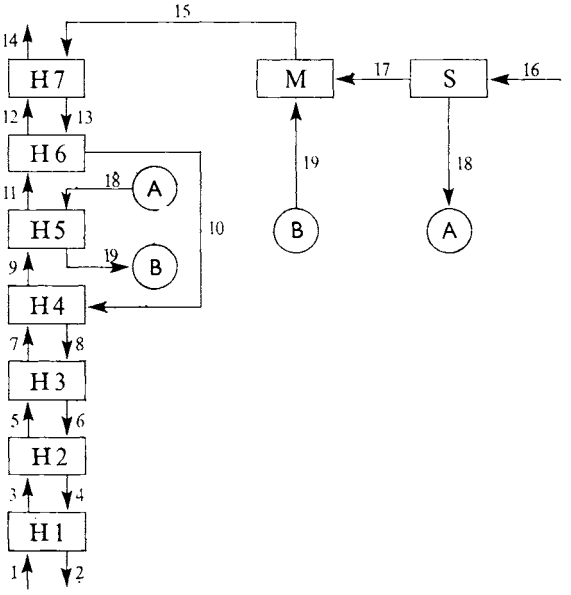


FIG. 2

Flowchart of xylene cooling by mother liquor. H heat exchanger, M mixer, S splitter

in a topological concept, requires the reformulation of the element models, which was performed on chemical engineering basis, with REGULA FALSI being used as an iteration method. 5) Topology-oriented simulation using inverse information flow with the element models being established on the basis of global sensitivity studies. Successive iteration was used as an iteration method. 6) This variant is identical with the 5th one with the exception of the iteration method used. REGULA FALSI was employed. 7) Equation-oriented simulation, using the algorithm of RAMIREZ–VESTAL[15] for analyzing the set of equations which describes the overall chemical system, and a discretized regularized GAUSS–NEWTON procedure for the itera-

TABLE III

Results of the simulation of xylene cooling by mother liquor (distribution coefficient = 0·666)

| Stream | Temperature | Mass flow | Stream | Temperature | Mass flow |
|---|---|---|---|---|---|
| 1 | 315·15 | 11·125 | 11 | 255·96 | 11·125 |
| 2 | 311·82 | 9·250 | 12 | 243·52 | 11·125 |
| 3 | 307·59 | 11·125 | 13 | 244·59 | 9·250 |
| 4 | 302·57 | 9·250 | 14 | 241·15 | 11·125 |
| 5 | 296·35 | 11·125 | 15 | 234·75 | 9·250 |
| 6 | 289·57 | 9·250 | 16 | 221·15 | 9·250 |
| 7 | 282·74 | 11·125 | 17 | 221·15 | 6·170 |
| 8 | 272·49 | 9·250 | 18 | 221·15 | 3·080 |
| 9 | 266·37 | 11·125 | 19 | 260·09 | 3·080 |
| 10 | 252·39 | 9·250 | | | |

TABLE IV

Results of the simulation of xylene cooling by mother liquor (elements)

| Heat exchanger | Amount of heat transferred $kJ\,s^{-1}$ | Area $m^2$ | Overall heat transfer coefficient $kJ\,s^{-1}\,m^{-2}\,K^{-1}$ |
|---|---|---|---|
| 1 | 148·376 | 148·76 | 245·29 |
| 2 | 205·615 | 148·76 | 231·08 |
| 3 | 264·425 | 148·76 | 205·88 |
| 4 | 301·681 | 148·76 | 168·69 |
| 5 | 187·546 | 35·61 | 316·08 |
| 6 | 114·336 | 148·76 | 182·52 |
| 7 | 142·029 | 148·76 | 165·87 |

tion of the system (GOS–84 programsystem). *8*) Equation-oriented simulation, using a global sensitivity algorithm in the analysis of the set of equations and successive iteration as an iteration procedure (GOS–84 system).

Element programs based on chemical engineering considerations resulted in a divergent behaviour when internal iteration by a successive iteration procedure was used. Consequently, this variant is not considered in this paper. To confirm the information content of the results, the calculation was carried out for all variants mentioned above with three different sets of data as starting values for the iteration. The results of the investigation are summarized in Table V. The eight computational variants of solution were compared with respect to the following items: *1*) Number of iterations over the system (ITS). In the topology-oriented system, external iteration over the overall chemical system is carried out by the successive iteration procedure. *2*) Average number of iterations in the elements (ITE). This value is of importance only in the topology-oriented approach. Using these data, comparison of the individual variants may yield information about the quality of internal iterations in the elements. *3*) Computing time (in seconds) required for the solution (RZL). In the com-

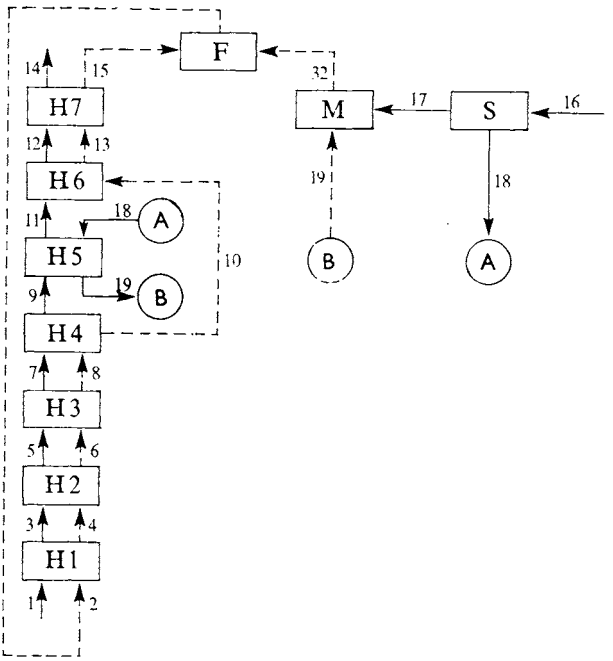


FIG. 3

Flowchart of xylene cooling by mother liquor with inverse information flow. H heat exchanger, M mixer, S splitter, F fictive node

parison of computing times for the solution between topology-oriented and equations-oriented simulation it must be borne in mind that the GOS–84 system, at the time the comparative calculation was carried out, did not involve any rearrangement of equations. The individual equation were solved by determining the zeroes according to NEWTON. The possibility of rearrangement which now exists decreases the computing time to about one third.

As has been expected, the variants solved by inverse information flow (4, 5, 6) gave more favourable results than those calculated according to the topological direction of flow (1, 2,3). Comparison of variants 1 and 4 reveals that inverse information flow may result in a 50 per cent saving of computing time. It must be emphasized, however, that inverse information flow in topology-oriented program systems involves considerable difficulties, as in this case there are hardly any standard models available.

The significance of the strategy of modelling with models for topology-oriented systems is evident from the comparison between variants 1 and 3 as well as between 4 and 6. Both cases show that a purely technological approach is not necessarily the most favourable principle. Rather, it appears to be necessary to consider system engineering aspects, as is evident from variants 2, 3, 5, and 6.

Comparison between equation-oriented variants and topology-oriented variants is quite interesting. From the point of overall computing time (RZG), the equation-oriented simulation appears to be little suited for solving the examples mentioned above. The computing time required for the solution, however, appears to be another thing. With the exception of the computational variants 5 and 6, which in conse-

TABLE V
Results of the investigation of the computational variants

| Variant | Set of data 1 | | | | Set of data 2 | | | | Set of data 3 | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | ITS[a] | ITE[b] | RZL[c] | RZG[d] | ITS | ITE | RZL | RZG | ITS | ITE | ZRL | RZG |
| 1 | 102 | 6 | 131 | 141 | 99 | 6 | 119 | 129 | 97 | 5 | 108 | 118 |
| 2 | 139 | 3 | 108 | 118 | 142 | 3 | 118 | 128 | 114 | 3 | 100 | 110 |
| 3 | 109 | 4 | 109 | 119 | 108 | 4 | 94 | 104 | 74 | 4 | 70 | 80 |
| 4 | 11 | 38 | 61 | 71 | 11 | 38 | 73 | 83 | 9 | 41 | 55 | 65 |
| 5 | 7 | 26 | 30 | 40 | 7 | 26 | 30 | 40 | 7 | 26 | 32 | 42 |
| 6 | 9 | 8 | 33 | 43 | 9 | 8 | 28 | 38 | 9 | 8 | 28 | 38 |
| 7 | 3 | — | 39 | 291 | 3 | — | 40 | 292 | 3 | — | 43 | 300 |
| 8 | 61 | — | 72 | 467 | 62 | — | 84 | 496 | 55 | — | 78 | 456 |

[a] Number of iterations over the system; [b] average number of iterations in an element; [c] computing time required for the solution (seconds); [d] total computing time (seconds).

quence of inverse information flow as well as of the special strategy of modelling on the basis of sensitivity theoretical studies, are very expensive with respect to modelling, the computational variants 7 and 8, which represent the equation-oriented simulation, yield the most favourable results. Hence, it follows that the equation-oriented approach apart from being very adaptable is most promising for problems requiring repeated calculation of the system (*e.g.* optimization and consideration of parameter uncertainties). The difference between RZG and ZRL corresponds to the computing time used for analysis and generation of the simulation problem which in the case of repeated calculation is required only once.

The main advantages of the equation-oriented simulation approach can be summarized as follows: *1*) By removing the elements boundaries (natural for topological simulation concept) it is possible to formulate the hierarchy and sequence of solution so that the problem is solved with the highest efficiency. The equation-oriented approach allows any problem to be of arbitrary formulation and internal mathematical structure. *2*) The flexibility of the equation-oriented simulator according to the role of individual variables enables us to formulate various technological problems in different ways without substantial programming effect. *3*) It is possible to utilize the free concept of all variables of the system for its optimization. From this point it is not necessary to differentiate among individual variables and even among individual technological streams as for their orientation.

It is then possible to solve the dual form of the problem in common with the primary one.

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