GLOBAL STEADY STATE SIMULATION OF COMPLEX TECHNOLOGICAL SYSTEMS — AN UNIFIED APPROACH

Josef VRBA

Institute of Chemical Process Fundamentals, Czechoslovak Academy of Sciences, 165 02 Prague - Suchdol

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In general, mathematical models of steady state simulation schemas of complex technological processes are formed by sets of algebraic equations. The formal description of global approach to the solution of such sets is presented. The utilization of preliminary solution of linear equations of the set for its reduction and for the expression of dependency of the so-called eliminated variables on the remaining ones, as arguments of the reduced set, (*i.e.* the first decomposition level) is considered. The determination of disjoint subsystems of the reduced set (*i.e.* the subsets of nonlinear equations which may be solved serially and independently of each other in a sequence) and the determination of the hierarchy of their solution, when there are several such subsystems, is meant as the second decomposition level. The possibility of including of special models with particular computational algorithms in the equation-like model of complex system and the way of solution of such a problem with the mentioned two-level decomposition is also discussed. The including of both types of decomposition and the solution of the reduced set of equations in common computational block is dealt with.

The mathematical model of a steady state simulation schema of complex technological process is in general formed by a mixed consistent set of linear and nonlinear algebraic equations of N variables

$$f_i(\mathbf{X}) \equiv \sum_{j=1}^{N} a_{ij} x_j + c_i = 0 \; ; \quad i = 1, \ldots, M \tag{1}$$

$$f_k(\mathbf{X}) \equiv f_k(x_1, \ldots, x_N) = 0 \; ; \quad k = M + 1, \ldots, L \leqq N \, . \tag{2}$$

In particular cases, the necessity to describe the process in some parts of its complete schema by other form than by equations (*1*) or (*2*) may be met during the construction of the model. Then we assume that this form is solved out of the set (1), (2) and its connection with the set is intermediated by an auxiliary transcription, formally consistent with this set. For the schemas of complex processes it is typical that the matrix of coefficients a_{ij} of the linear subset (1) is sparse, the occurrence of individual variables x_j in the nonlinear subset (*2*) is sparse as well. Moreover, the number of linear equations as usual exceeds significantly the number of nonlinear equations

(basing on experience we know that from the total number of equations (*1*), (*2*) almost 80% are often of the type (1)). These facts force us to consider to apply the decomposition techniques for the solution of the set (1), (2).

The decomposition enables significant reduction in the number of equations and variables for the solution itself (mostly of iterative character). It makes also possible the forming of a set of subsystems of simultaneous equations, which is important for accuracy and convergency of the computation. As far as the individual phases of the computation are realized separately, the reduction in requirements on computer storage is the significant result of decomposition. In this paper, all computational phases are followed in their continuous relationship without the necessity of interruption and "hand" intervention into the computational process.

The first level of decomposition concerns the reduction of the dimensionality of the set (1), (2). For the formulation of the reduced set, represented only by the nonlinear equations (*2*), the linear subset (1) is utilized. There are M properly selected variables (so-called eliminated variables) expressed through the coefficients a_{ij} and the constants c_i in a relationship on $N-M$ remaining variables – *i.e.* the variables, which remain explicitly in the formed reduced set[1]. This step is performed only once without the necessity of repetition, the numerical relation between the eliminated variables and the remaining ones is expressed in the form of a simple functional coordination.

The distribution of the reduced set into disjoint subsystems and the determination of the hierarchy of their solution is understood as the second level of decomposition. A number of methods already exist for this purpose[2] of which that proposed by Steward[3] is considered as the most efficient. This method is used also in this paper. The second-level decomposition is performed only once, too.

It is useful to give some definitions and matrix notations, used throughout the further text, before starting with the description of individual steps of the solution of (1), (2):

$\{i\} \leftrightarrow i = 1, \ldots, M$ – the set $\{i\}$ is formed by elements of values $1, \ldots, M$

$\{m\} \subset \{i\} \leftrightarrow \{i \mid P\}$ – the set $\{m\}$ is formed by those elements of $\{i\}$ for which the property P exists

$\alpha_{(i)}$ – the subscript of the quantity α gets all values of the set $\{i\}$

$\xi \in \{i\} : \alpha_\xi = L(\alpha_{(i)})$ – for the element ξ of the set $\{i\}$ the relation L between the quantities α_ξ and $\alpha_{(i)}$ exists

$\sum_j Ba_j = \max_j (a_j)$ – Boolean sum of quantities a_j (a_j gets the values 0 or 1)

$\prod_j Ba_j = \min_j (a_j)$ – Boolean product of quantities a_j (a_j gets the values 0 or 1)

$\mathbf{B}(M, N) = (b_{ij})$ – the matrix $\mathbf{B}$ consists of elements b_{ij} ordered into M rows and N columns

Data for Computation

Data for computation are given in the following form:

N – number of variables of the set (1), (2)
L – number of equations of the set (1), (2)
M – number of linear equations (*1*)
$\mathbf{A}(M, N) = (a_{ij})$ – matrix of coefficients of linear equations (*1*)
$\mathbf{C}(M, 1) = (c_i)$ – vector of constants of linear equations (*1*)
$\mathbf{Q}(L - M, N) = (q_{kj})$ – occurrence matrix of nonlinear set (2), where

$$q_{kj} = \begin{cases} 1 \text{ in case of explicit occurrence of } x_j \text{ in } f_k(\mathbf{X}) = 0 \\ 0 \text{ otherwise} \end{cases}$$

$\mathbf{X}(N, 1) = (x_j)$ – vector of original variables of the set (1), (2). As data the starting approximations of x_j are used.

If for some variables the role of remaining variables is considered in advance (*e.g.* when they are to be treated as control variables – see later), a Boolean vector $\vartheta(N, 1) = (\vartheta_j)$ is introduced, where

$$\vartheta_j = \begin{cases} 1 \text{ if the variable } x_j \text{ is to be taken as the remaining one} \\ 0 \text{ otherwise} \end{cases}$$

It is assumed that there is no such equation in the subset (1), which contains as its explicite variables only those with $\vartheta_j = 1$ (the subset (1) degenerates in this case).

The particular form of nonlinear equations (*2*) is introduced as a special subprocedure.

Solution of the Subset of Linear Equations – Selection of Eliminated and Remaining Variables

The linear subset (1) may be written in a matrix form as:

$$\mathbf{AX} + \mathbf{C} = \mathbf{O}. \qquad (3)$$

In the properly formulated problem, the rank of the matrix **A** equals M, *i.e.* M variables x may be eliminated and expressed in a functional dependency on $N - M$ remaining variables. In the given context, the eliminated variables play the role of output variables and the remaining ones that of input variables of the subset (1), (3), respectively. The selection of eliminated variables is in general not unambiguous. As a rule, it must be performed not to give a chance for the degeneracy of (1) (*i.e.* the occurrence of only remaining variables in some equations of (*1*)). Moreover, we demand that the selection of eliminated variables must enable the maximal decomposition of the subset (1). This decomposition manifests itself in maximal grouping of coefficients a_{ij} along and on the main diagonal of the matrix formed by the columns of **A** consistent with the eliminated variables. The occurrence matrix

of the subset (1) $\mathbf{B}(M, N) = (b_{ij})$, where

$$b_{ij} = \begin{cases} 1 & \text{for } a_{ij} \neq 0, \\ 0 & \text{otherwise} \end{cases}$$

is constructed besides the matrix **A**.

A heuristic algorithm was prepared for the decomposition of the subset (1) and the elimination of variables:

Algorithm. 1.

A. $\{i\} \leftrightarrow i = 1, \ldots, M$
$\{j\} \leftrightarrow j = 1, .., N$
$\alpha_{\{i\}} = 0$
$\beta_j = \gamma_j = \begin{cases} 1 & \text{if } b_{\{i\}j} = 0 \text{ or } \vartheta_j = 1 \\ 0 & \text{otherwise} \end{cases}$

B. If $\sum_j \gamma_j = N - M$, continue with Step G.

C. $\{m\} \leftrightarrow \{i \mid \alpha_i = 0\}$
$\{n\} \rightarrow \{j \mid \beta_j = 0\}$
$\Theta_m = \sum_n b_{mn}$
$\{s\} \subset \{m\} : \Theta_s = \min_m [\Theta_m]$

D. If $\Theta_s > 1$, continue with Step F.

E. Let $\Theta_s = b_{sr}$, then $1 \rightarrow \alpha_s \rightarrow \beta_r$. Go back to Step C.

F. $\{\eta(s)\} \leftrightarrow \{j \mid (b_{sj} = 1) \cap (\beta_j = 0)\}$
$\{\xi[\eta(s)]\} \leftrightarrow \{i \mid (b_{i\eta(s)} = 1) \cap (\alpha_i = 0)\}$
$\psi_{\eta(s)} = \sum_n \sum_{\xi[\eta(s)]} B b_{\xi[\eta(s)]n} - \sum_{\xi[\eta(s)]} 1$
$\{r\} \subset \{\eta(s)\} : \psi_r = \max_{\eta(s)} [\psi_{\eta(s)}]$.

For arbitrary $r : 1 \rightarrow \beta_r \rightarrow \gamma_r$. Go back to Step B.

G. $\alpha_{\{1\}} = 0, \beta_{\{i\}} = 0$

H. $\{m\} \leftrightarrow \{i \mid \alpha_i = 0\}$
$\{n\} \leftrightarrow \{j \mid (\beta_j = 0) \cap (\gamma_j = 0)\}$
$\Theta_n = \sum_m b_{mn}$
$\{r\} \subset \{n\} : \Theta_r = \min_n [\Theta_n]$.

For arbitrary $r : \{k\} \leftrightarrow \{i \mid (\alpha_i = 0) \cap (b_{ir} = 1)\}$

$\psi_k = \sum_n b_{kn}$

$\{s\} \subset \{k\} : \psi_s = \min_k [\psi_k]$.

For arbitrary $s : r \to \alpha_s$, $1 \to \beta_r$

I. If $\alpha_{\{i\}} \neq 0$, continue with Step J. Otherwise go back to Step H.

J. $\{m\} \leftrightarrow \{i\}$, $\{n\} \leftrightarrow \{j\}$

$$\gamma_j = \beta_j \sum_{k=1}^{j} \beta_k + (1 - \beta_j)(M + j - \sum_{k=1}^{j} \beta_k)$$

$$u_{im} = \begin{cases} 1 & \text{for } \gamma_{\alpha_m} = i, \\ 0 & \text{otherwise} \end{cases} \qquad v_{nj} = \begin{cases} 1 & \text{for } \gamma_n = j. \\ 0 & \text{otherwise} \end{cases}$$

In Step A those x's of the variables of the linear subset (1) are excluded automatically, which do not explicitly occur in it and therefore cannot be used for its solution, or those determined in advance for the role of remaining variables. In Step B the decomposition of (1) is accomplished if there already $N - M$ variables have been selected.

In Step C a linear equation with the smallest occurrence of variables, not excluded up to this step, is selected. An equation with only one such variable represents an independent subsystem in (1) on given level of the hierarchy of solution and may be excluded from further considerations on decomposition. The respective variable remains as the variable of the subset (1) and further it does not play the role of explicit variable of the subset (2). When there are several variables in the selected equation, the number of degrees of freedom of the respective subsystems, consistent with this equation according to its individual variables, is determined. The variable, which corresponds with the subsystem with the greatest number of degrees of freedom, is excluded from the subset (1) – it becomes the explicit variable of the subset (2) (Step F). In case of several equations with the smallest occurrence of variables, we explore in this way all the variables of these equations. If there are several variables with maximal number of degrees of freedom, an arbitrary one of such variables is excluded. By the number of degrees of freedom of a subsystem the number of variables minus the number of equations is understood at this place. In this way, we preserve for the subset (1) the variables, for which it is necessary to solve subsystems of smallest dimensions and exclude those, which correspond with subsystems of largest dimensions. Thus, the possibility of formation of the greatest number of subsystems is explored. As for the linear subset (1), we are directly interested neither in the hierarchy of formed subsystems nor in their internal structure. The decomposition manifests here itself by the efficient grouping of coefficients a_{ij} along and on the main diagonal of the first M columns of the reorganized matrix **A**. The described way of

decomposition is maximaly efficient but not necessarily unambiguous. The variables, which are excluded from the linear subset (1) in Steps A-H, are the remaining variables with explicit occurrence in the nonlinear equations of the subset (2).

Now, it is necessary to reorganize the subset (1) with respect to its solution for the eliminated variables on the one hand and with respect to the relation between these variables and the remaining ones on the other. This is performed in the second part of Algorithm 1. (Steps G-J). The matrices of row and column rearrangements of $\mathbf{A}$ and $\mathbf{C}$, *i.e.* $\mathbf{U}(M, M) = (u_{im})$ and $\mathbf{V}(N, N) = (v_{nj})$, represent the results. By the help of $\mathbf{U}$ and $\mathbf{V}$, the transformation between the original variables vector $\mathbf{X}(N, 1)$, the eliminated variables vector $\mathbf{Y}_E(M, 1)$ and the remaining variables vector $\mathbf{Y}_R(N - M, 1)$ is expressed. Both matrices $\mathbf{U}$ and $\mathbf{V}$ are the orthogonal ones, so that the relations

$$\mathbf{U}^{-1} = \mathbf{U}^T \tag{4}$$

$$\mathbf{V}^{-1} = \mathbf{V}^T \tag{5}$$

and the relations between $\mathbf{Y}$ and $\mathbf{X}$, *i.e.*

$$\mathbf{Y} = (\mathbf{Y}_E^T, \mathbf{Y}_R^T)^T = \mathbf{V}^T\mathbf{X} \tag{6}$$

$$\mathbf{X} = \mathbf{V}\mathbf{Y} \tag{7}$$

are valid. If we denote the first M columns of $\mathbf{V}$ as a matrix $\mathbf{V}_E(N, M) = (v_{ji}^E)$ and the remaining $N - M$ columns as a matrix $\mathbf{V}_R'(N, N - M) = (v_{jk}^R)$ $(i = 1, \ldots, M, k = M + 1, \ldots, N, j = 1, \ldots, N)$, then

$$\mathbf{X} = (\mathbf{V}_E, \mathbf{V}_R)(\mathbf{Y}_E^T, \mathbf{Y}_R^T) = \mathbf{V}_E\mathbf{Y}_E + \mathbf{V}_R\mathbf{Y}_R\,. \tag{8}$$

The left-hand multiplication of Eq. (3) by $\mathbf{U}$ and the substitution of (8) for $\mathbf{X}$ lead to the equation

$$\mathbf{U}\mathbf{A}(\mathbf{V}_E\mathbf{Y}_E + \mathbf{V}_R\mathbf{Y}_R) + \mathbf{U}\mathbf{C} = \mathbf{O}\,, \tag{9}$$

from where the relation between the eliminated variables and the remaining ones

$$\mathbf{Y}_E = -(\mathbf{A}_U\mathbf{Y}_R + \mathbf{C}_U)\,, \tag{10}$$

where

$$\mathbf{A}_U(M, N - M) = (a_{ik}^U) = (\mathbf{U}\mathbf{A}\mathbf{V}_E)^{-1}\,\mathbf{U}\mathbf{A}\mathbf{V}_R \tag{11}$$

$$\mathbf{C}_U(M, 1) = (c_i^U) = (\mathbf{U}\mathbf{A}\mathbf{V}_E)^{-1}\,\mathbf{U}\mathbf{C} \tag{12}$$

and the relation between the original and the remaining variables

$$\mathbf{X} = -(\mathbf{A}_V \mathbf{Y}_R + \mathbf{C}_V), \tag{13}$$

where

$$\mathbf{A}_V(N, N - M) = (a_{jk}^V) = \mathbf{V}_E \mathbf{A}_U - \mathbf{V}_R \tag{14a}$$

$$\mathbf{C}_V(N, 1) = (c_j^V) = \mathbf{V}_E \mathbf{C}_U \tag{14b}$$

$$i = 1, \ldots, M$$

$$k = M + 1, \ldots, N$$

$$j = 1, \ldots, N$$

can be obtained. At the same time the vector

$$\vartheta_R(N - M, 1) = (\vartheta_k^R) = \mathbf{V}_R^T \vartheta \tag{15}$$

is calculated (if necessary). The explicit occurrence of the original variables x in the non-linear subset (2) is indicated by the occurrence matrix $\mathbf{Q}(L - M, N)$. Knowing the form of dependence between eliminated and remaining variables, we can construct a reduced occurrence matrix $\mathbf{Q}_R(L - M, N - M)$, indicating the occurrence of only the remaining variables in (2). By the help of the matrix $\mathbf{A}_V$, we construct the auxiliary matrix of coincidence of eliminated and remaining variables $\mathbf{W}(N, N - M) = (w_{jk})$, where

$$w_{jk} = \begin{cases} 1 & \text{for } a_{jk}^V \neq 0 . \\ 0 & \text{otherwise} \end{cases}$$

The reduced occurrence matrix $\mathbf{Q}_R$ is now given by the relation

$$\mathbf{Q}_R = (q_{lk}^R) = \mathbf{QW}, \quad l = M + 1, \ldots, L; \; k = M + 1, \ldots, N, \tag{16}$$

where the Boolean arithmetics is used. Up to this step of computation, all information concerning the set (1), (2) and the transformation of variables are concentrated in the matrices $\mathbf{A}_V$, $\mathbf{Q}_R$ and the vectors $\mathbf{C}_V$, $\mathbf{X}$, $\mathbf{Y}_R$.

Solution of the Subset of Nonlinear Equations — Selection of Iterated and Control Variables

For the selection of independent subsystems of a set of algebraic equations and the determination of hierarchy of their solution, the method based on the theory of graphs was developed by Steward[3]. The principle aim of the method is to determine an output variable in each equation of the set, for which the equation can be solved provided

we know the values of all other variables, occurring explicitly in the equation. At the same time, it is assumed that the set of equations is consistent and definite. In our case, this assumption means that $L = N$, *i.e.* the matrix $\mathbf{Q}_R$ is a $(N - M)$ square matrix.

In general case, when $L < N$, it is necessary to exclude $N - L$ variables from the set of remaining variables (represented by the vector $\mathbf{Y}_R$). The values of these excluded variables must be given in advance for the solution of equations (2) (*e.g.* the values are determined in the frame of an optimization procedure or given as particular parameters of the simulated process). Let us formally call these variables as control variables $\mathbf{Z}_C(N - L, 1)$ and the other variables of $\mathbf{Y}_R$ as iterated variables $\mathbf{Z}_I(L - M, 1)$, For the selection of control variables similar heuristic algorithm, as that described in the preceding part, can be used:

Algorithm 2.

A. $\{i\} \leftrightarrow i = M + 1, \ldots, L$
$\{j\} \leftrightarrow j = M + 1, \ldots, N$
$\alpha_{\{i\}} = 0$
$\beta_j = \gamma_j = \begin{cases} 1 & \text{if } \vartheta_j^R = 1 \\ 0 & \text{otherwise} \end{cases}$

B. If $\sum_j \gamma_j = N - L$, continue with Step G.

C. $\{m\} \leftrightarrow \{i \mid \alpha_i = 0\}$
$\{n\} \leftrightarrow \{j \mid \beta_j = 0\}$
$\Theta_m = \sum_n q_{mn}^R$
$\{s\} \subset \{m\} : \Theta_s = \min_m [\Theta_m]$

D. If $\Theta_s > 1$, continue with Step F.

E. Let $\Theta_s = q_{sr}^R$, then $1 \to \alpha_s \to \beta_r$. Go back to Step C.

F. $\{\eta(s)\} \leftrightarrow \{j \mid (q_{sj}^R = 1) \cap (\beta_j = 0)\}$
$\{\xi[\eta(s)]\} \leftrightarrow \{i \mid (q_{i\eta(s)}^R = 1) \cap (\alpha_i = 0)\}$
$\psi_{\eta(s)}(s) = \sum_n \sum_{\xi[\eta(s)]} B q_{\xi[\eta(s)]n}^R - \sum_{\xi[\eta(s)]} 1$
$\{r\} \subset \{\eta(s)\} : \psi_r = \max_{\eta(s)} [\psi_{\eta(s)}(s)]$
For arbitrary $r : 1 \to \beta_r \to \gamma_r$. Go back to Step B.

G. $\alpha_{\{i\}} = 0$, $\beta_{\{j\}} = 0$

H. $\{m\} \leftrightarrow \{i \mid \alpha_i = 0\}$

$\{n\} \leftrightarrow \{j \mid (\beta_j = 0) \cap (\gamma_j = 0)\}$

$\Theta_n = \sum_m q^R_{mn}$

$\{r\} \subset \{n\} : \Theta_r = \min_n [\Theta_n]$

For arbitrary $r : \{k\} \leftrightarrow \{i \mid (\alpha_i = 0) \cap (q^R_{ir} = 1)\}$

$\psi_k = \sum_n q^R_{kn}$

$\{s\} \subset \{k\} : \psi_s = \min_k [\psi_k]$

For arbitrary $s : r \to \alpha_s, 1 \to \beta_r$

I. If $\alpha_{\{i\}} \neq 0$, continue with Step J. Otherwise go back to Step H.

J. $\{m\} \leftrightarrow \{i\}, \{n\} \leftrightarrow \{j\}$

$$\gamma_j = \beta_j(M + \sum_{k=M+1}^{j} \beta_k) + (1 - \beta_j)(L - M + j - \sum_{k=M+1}^{j} \beta_k)$$

$$e_{mi} = \begin{cases} 1 & \text{for } \gamma_{\alpha_m} = i \\ 0 & \text{otherwise} \end{cases}, \quad d_{nj} = \begin{cases} 1 & \text{for } \gamma_n = j \\ 0 & \text{otherwise} \end{cases}$$

The result of the described procedure is the construction of the orthogonal matrix $\mathbf{D}(N - M, N - M) = (d_{nj})$, which plays similar role as the matrix $\mathbf{V}$ for the transformation $\mathbf{Y} \leftrightarrow \mathbf{X}$, and the matrix of output variables $\mathbf{E}(L - M, L - M) = (e_{mi})$. Then

$$\mathbf{Z}(N - M, 1) = (\mathbf{Z}_I^T, \mathbf{Z}_C^T)^T = \mathbf{D}^T\mathbf{Y}_R \qquad (17)$$

and

$$\mathbf{Y}_R = \mathbf{D}\mathbf{Z} . \qquad (18)$$

Let the first $L - M$ columns of the matrix $\mathbf{D}$ form a matrix $\mathbf{D}_I$ and the other $N - L$ columns a matrix $\mathbf{D}_C$, then

$$\mathbf{Y}_R = (\mathbf{D}_I, \mathbf{D}_C)(\mathbf{Z}_I^T, \mathbf{Z}_C^T)^T = \mathbf{D}_I\mathbf{Z}_I + \mathbf{D}_C\mathbf{Z}_C \qquad (19)$$

(the dimensions of $\mathbf{D}_I$, $\mathbf{D}_C$ are $(N - M, L - M)$, $(N, N - L)$, respectively). The resulting occurrence matrix for the nonlinear set $\mathbf{Q}_I(L - M, L - M) = (q^I_{im})$ $(i = m = M + 1, \ldots, L)$ is determined by the relation:

$$\mathbf{Q}_I = \mathbf{Q}_R\mathbf{D}_I . \qquad (20)$$

Using the output variables matrix $\mathbf{E}$ and the occurrence matrix $\mathbf{Q}_I$, we may construct the adjacency matrix (*i.e.* the Boolean matrix that shows the flow of informa-

tion between equations) $\mathbf{P}(L - M, L - M) = (p_{\mathrm{im}})$ according to the relation:

$$\mathbf{P} = \mathbf{E}\mathbf{Q}_{\mathrm{I}}^{\mathrm{T}} . \tag{21}$$

The matrix $\mathbf{E}$ contains in any row and column only one non-zero element $e_{\mathrm{mi}} = 1$ if the i-th variable is the output variable of the m-th equation. Then (in accordance with (21)), an element of $\mathbf{P}$ (*i.e.* p_{mi}) equals 1 only if the output variable of the m-th equation explicitly occurs in the i-th equation, otherwise $p_{\mathrm{mi}} = 0$. The form of the adjacency matrix $\mathbf{P}$ depends on the way of construction of the matrix $\mathbf{E}$. According to its character, the adjacency matrix $\mathbf{P}$ corresponds with the associated matrix known from the theory of graphs. The individual equations of the solved set (2) correspond with nodes and the variable z_j ($j = M + 1, \ldots, L$), organized in the vector $\mathbf{Z}_{\mathrm{I}}$, with flows of an oriented (generaly cyclic) graph. The indication of the occurrence of oriented chains in a graph by the help of its Boolean powers does represent the significant property of associated matrix. In our case, these oriented chains correspond with the chains of succesive substitution of values of variables from one equation into other. For $L - M$ equations of the subset (2), the $(L - M)$-th Boolean power of $\mathbf{P}$ (*i.e.* $\mathbf{P}^{(L-M)} = (p_{\mathrm{mi}}^{(L-M)})$) indicates the common occurrence of m-th and i-th equations in a subsystem if and only if

$$p_{\mathrm{mi}}^{(L-M)} = p_{\mathrm{im}}^{(L-M)} = 1 . \tag{22}$$

The condition (2) expresses the simultaneous existence of the chain of succesive substitution from m-th equation into the i-th one and on the contrary. Thus, the final result of decomposition doesn't depend on the way of construction of the matrix $\mathbf{E}$. At the same time, by the condition (22) the procedure for the determination of individual subsystems of (2) is given. The following algorithm is given for the construction of a matrix $\mathbf{G}(L - M, L - M) = (g_{\mathrm{mi}})$:

Algorithm 3.

A. $\{m\} \leftrightarrow \{i\} \leftrightarrow m,\ i = M + 1, \ldots, L$
$g_{\mathrm{(m)(i)}} = 0$
$M + 1 \rightarrow l$

B. $\{r\} \leftrightarrow \{m \mid g_{\mathrm{(i)m}} = 0\}$

C. If $l \notin \{r\}$, continue with Step E.

D. $\{s\} \leftrightarrow \{r \mid p_{\mathrm{rl}}^{(L-M)} = p_{\mathrm{lr}}^{(L-M)} = 1\}$
$1 \rightarrow g_{\mathrm{l(s)}}$

E. $l + 1 \rightarrow l$

F. If $l \leqq L$, go back to Step B, otherwise the construction of $\mathbf{G}$ is accomplished.

It is generaly valid for powers of $\mathbf{P}$ that $\mathbf{P}^{(m)} = \mathbf{P}^{(L-M)}$ for $m \geqq L - M$, therefore it is possible to use the recurrent formula

$$\mathbf{PP} \to \mathbf{P}^{(2)}, \mathbf{P}^{(2)}\mathbf{P}^{(2)} \to \mathbf{P}^{(4)}, \ldots, \mathbf{P}^{(k)}\mathbf{P}^{(k)} \to \mathbf{P}^{(2k)} \tag{23}$$

as long as $2k < L - M$. In cases, when the maximal number of equations in one subsystem is less than $L - M$, we find that $\mathbf{P}^{(m)} = \mathbf{P}^{(L-M)}$ for $1 \leqq m < L - M$. In the extreme case, when any equation of (2) itself represents a subsystem, $\mathbf{P}^{(L-M)} = \mathbf{P}$. It is therefore usefull to finish the procedure (23) just after $\mathbf{P}^{(2k)} = \mathbf{P}^{(k)}$.

Any row of the matrix $\mathbf{G}$ represents a list of those equations from (2), which occur in the subsystem corresponding with the row. If some subsystem consists of more than one equation, some of rows of $\mathbf{G}$ contain only zero elements. The number of non-zero rows gives the number of subsystems with subscripts $\{s\} \leftrightarrow s = 1, \ldots, S$ $(1 \leqq S \leqq L - M)$, if no decomposition of (2) is possible, then $S = 1$. The equation $f_i(\mathbf{X}) = 0$ is the equation of the s-th subsystem if $g_{si} = 1$. When excluding the zero rows from the matrix $\mathbf{G}$, we obtain a matrix $\hat{\mathbf{G}}(S, L - M) = (\hat{g}_{si})\,(i = M + 1, \ldots, L)$.

By substitution of (19) into (13), the transformation relations between original variables x, iterated variables z^I and control variables z^C can be gained, *i.e.*

$$\mathbf{X} = -(\mathbf{H}_I\mathbf{Z}_I + \mathbf{H}_C\mathbf{Z}_C + \mathbf{C}_V) = -(\mathbf{HZ} + \mathbf{C}_V)\,, \tag{24a}$$

where the relation for the matrices $\mathbf{H}_I(N, L - M)$, $\mathbf{H}_C(N, N - L)$ and $\mathbf{H}(N, N - M)$ of the form

$$(\mathbf{H}_I, \mathbf{H}_C) = (\mathbf{A}_V\mathbf{D}_I, \mathbf{A}_V\mathbf{D}_C) = \mathbf{A}_V\mathbf{D} = \mathbf{H} = (h_{jk})\,. \tag{24b}$$

$$j = 1, \ldots, N$$

$$k = M + 1, \ldots, N$$

is valid. Up to this step of computation, all information necessary for the solution of the set (1), (2) are concentrated in the matrices $\mathbf{H}$, $\hat{\mathbf{G}}$ and the vectors $\mathbf{C}_V$, $\mathbf{Z}$, $\mathbf{X}$. The matrix $\hat{\mathbf{G}}$ itself doesn't determine the hierarchy (*i.e.* order of solution sequence) of individual subsystems. As the first in the sequence only such a subsystem may be solved, in which the number of variables from $\mathbf{Z}_I$ equals the number of equations. There can be several of such subsystems, then the hierarchy of them is irrelevant. When determining the number of variables in up to now unsolved subsystems, we do not consider the variables of the subsystems, which have been solved – their final values are already known. We follow the rule: the solution of the s-th subsystem is preceded by the solution of the s'-th subsystem, if there exists a chain of succesive

substitution from the equations of the s'-th subsystem into the equations of the s-th subsystem (but not on the contrary, because both subsystems would then necessarily belong to the same subsystem). For the determination of the variables of individual subsystems we construct (by the use of Boolean arithmetics) the matrix $\mathbf{T}(S, L - M) = (t_{sj})$ using the relation:

$$\mathbf{T} = \hat{\mathbf{G}}\mathbf{Q}_{\mathrm{I}} . \tag{25}$$

The individual rows of the matrix $\mathbf{T}$ are the lists of variables z in corresponding subsystems (of course these variables are only the iterated ones). The solvability condition for the s-th subsystem on given level of hierarchy of solution is expressed by the formula

$$\Theta_s = \sum_r t_{sr} - \sum_j \hat{g}_{sj} \stackrel{!}{=} 0 \tag{26}$$

where $j = M + 1, \ldots, L$ and $\{r\}$ is the set of subscripts of variables from the vector $\mathbf{Z}_{\mathrm{I}}$, the values of which haven't been yet on the preceding levels of the hierarchy of solution determined. The solution of the subset (2) describes

Algorithm 4.

A. $\{j\} \leftrightarrow j = M + 1, \ldots, L$
$\{s\} \leftrightarrow s = 1, \ldots, S$
$\alpha_{(s)} = 0, \beta_{(j)} = 0$

B. $\{r\} \leftrightarrow \{j \mid \beta_j = 0\}$
$1 \rightarrow s$

C. If $\alpha_s = 1$, continue with Step E.

D. $\Theta_s = \sum_r t_{sr} - \sum_j \hat{g}_{sj}$
If $\Theta_s = 0$, continue with Step G.

E. $s + 1 \rightarrow s$

F. If $s \leqq S$, go back to Step C, otherwise the computation is finished.

G. $\{m\} \leftrightarrow \{j \mid \hat{g}_{sj} = 1\}$
$\{n\} \leftrightarrow \{r \mid t_{sr} = 1\}$

Solve the s-th subsystem of equations $f_{(m)}(\mathbf{X}) = 0$ for the variables $z_{(n)}$. After the solution of the s-th subsystem $1 \rightarrow \alpha_s \rightarrow \beta_{(n)}$. Go back to Step B.

All arithmetic operations, necessary for the solution of sets of nonlinear algebraic equations, are performed on the equations $f_{(m)}(\mathbf{X}) = 0$ and the variables $z_{(n)}$ only.

The operative transformation

$$\hat{\mathbf{X}} = -(\mathbf{H}\hat{\mathbf{Z}} + \mathbf{C}_V), \tag{27}$$

where $\hat{\mathbf{X}}$, $\hat{\mathbf{Z}}$ are the momentary values of the vectors $\mathbf{X}$, $\mathbf{Z}$, is used for this purpose.

The Transformation of Trivial Constraints

As the consequence of nonlinearity of Eqs (2), the set (1), (2) has in general more than one real solution. If $L = N$, the attainment of a particular solution depends on a certain starting approximation of $\mathbf{X}$ and possible utilizing of trivial constraints

$$\mathbf{X}_L \leqq \mathbf{X} \leqq \mathbf{X}_U, \tag{28}$$

where $\mathbf{X}_L$, $\mathbf{X}_U$ are the vectors of acceptable the least and the highest values of variables x in the area of possible occurrence of the seeked solution. The conditions (28) can also exist in an optimization problem, when $L < N$ (nontrivial constraints are supposed to be transferred by the help of the so-called slack variables in the form of (1) or (2) – see the reference[5]).

From the properties of the matrices $\mathbf{V}$ and $\mathbf{D}$ the following important relations result:

$$\mathbf{V}_R^T\mathbf{V}_E = \mathbf{O} \tag{29}$$

$$\mathbf{V}_R^T\mathbf{V}_R = \mathbf{I}_{N-M} \tag{30}$$

$$\mathbf{D}_I^T\mathbf{D}_C = \mathbf{O} \tag{31}$$

$$\mathbf{D}_I^T\mathbf{D}_I = \mathbf{I}_{L-M} \tag{32}$$

$$\mathbf{D}_C^T\mathbf{D}_I = \mathbf{O} \tag{33}$$

$$\mathbf{D}_C^T\mathbf{D}_C = \mathbf{I}_{N-L}. \tag{34}$$

Substituting the relations (14), (15) and (18) into (13), we get the relation

$$\mathbf{X} = -[(\mathbf{V}_E\mathbf{A}_U - \mathbf{V}_R)\,\mathbf{DZ} + \mathbf{V}_E\mathbf{C}_U] \tag{35}$$

and by the help of (35) and (28) (after some rearrangement) the inequalities

$$\mathbf{X}_L + \mathbf{V}_E\mathbf{C}_U \leqq -(\mathbf{V}_E\mathbf{A}_U - \mathbf{V}_R)\,\mathbf{DZ} \leqq \mathbf{X}_U + \mathbf{V}_E\mathbf{C}_U. \tag{36}$$

If we multiply the last inequalities from the left by the transposed matrix $\mathbf{V}_R$, then (with regard to (*29*) and (*30*)) the inequalities

$$\mathbf{V}_R^T\mathbf{X}_L \leqq \mathbf{DZ} \leqq \mathbf{V}_R^T\mathbf{X}_U \tag{37}$$

or (with regard to (*19*))

$$\mathbf{V}_R^T\mathbf{X}_L \leqq \mathbf{D}_I\mathbf{Z}_I + \mathbf{D}_C\mathbf{Z}_C \leqq \mathbf{V}_R^T\mathbf{X}_U \tag{38}$$

can be obtained. By the successive left hand side multiplication of the inequalities (*37*), (*38*) by the transposed matrices $\mathbf{D}$, $\mathbf{D}_I$ and $\mathbf{D}_C$, the trivial constraints of iterated and control variables are obtained (with regard to (*31*)–(*34*)) in the forms

$$\mathbf{Z}_L \leqq \mathbf{Z} \leqq \mathbf{Z}_U \tag{39}$$

$$\mathbf{Z}_{IL} \leqq \mathbf{Z}_I \leqq \mathbf{Z}_{IU} \tag{40a}$$

$$\mathbf{Z}_{CL} \leqq \mathbf{Z}_C \leqq \mathbf{Z}_{CU}\,, \tag{40b}$$

where

$$\mathbf{Z}_L = \mathbf{D}^T\mathbf{V}_R^T\mathbf{X}_L \tag{41}$$

$$\mathbf{Z}_U = \mathbf{D}^T\mathbf{V}_R^T\mathbf{X}_U \tag{42}$$

$$\mathbf{Z}_{IL} = \mathbf{D}_I^T\mathbf{V}_R^T\mathbf{X}_L \tag{43a}$$

$$\mathbf{Z}_{IU} = \mathbf{D}_I^T\mathbf{V}_R^T\mathbf{X}_U \tag{43b}$$

$$\mathbf{Z}_{CL} = \mathbf{D}_C^T\mathbf{V}_R^T\mathbf{X}_L \tag{44a}$$

$$\mathbf{Z}_{CU} = \mathbf{D}_C^T\mathbf{V}_R^T\mathbf{X}_U\,. \tag{44b}$$

Special Computational Algorithm Modules of the Simulated Process

We are often confronted with the cases, where it seems unproper or is even impossible to include the mathematical model of some part of the process directly into the set of equations (*1*), (*2*), when simulating complex technological processes. It is caused by the facts that such models are solved by closed algorithms of special character or are represented by sets of differential equations, etc. In the sense of process modelling, any such model can be formally understood as a set of transformation relations

$$\mathbf{F}(\mathbf{X}_{in}, \mathbf{X}_{out}) = \mathbf{O}\,, \tag{45}$$

where $\mathbf{X}_{in}$ is the vector of input variables and $\mathbf{X}_{out}$ the vector of output variables of the given module (a part of the process), which is described in this manner. There may be obviously a whole set of another variables, which represents the transformated information between the elements of $\mathbf{X}_{in}$ and those of $\mathbf{X}_{out}$ (distillation column or extraction cascade are the examples) but, in the sense of the model (*45*), we are not directly interested in them – they are the internal variables of the model and are interpreted in the frame of it only. On the other hand, the elements of $\mathbf{X}_{in}$ and $\mathbf{X}_{out}$ must necessarily be the variables of the overall model (*1*), (*2*). The possible way of how to connect the solution of the model (*45*) with the solution of the set of equations (*1*), (*2*) is to formulate a so-called representative model. That is of the type

$$\mathbf{X}_{out} = \Phi_{out/in}\mathbf{X}_{in}\,, \tag{46}$$

where $\Phi_{out/in}$ is a matrix of pseudoconstant parameters of the representative model, the values of which are corrected by the solution of the rigorous model (*45*). The individual equations of the model (*46*) are of the pseudolinear form

$$-x_\xi + \varphi_{\xi\eta}x_\eta = 0 \tag{47}$$

and represent at the same time the other definition for $\varphi_{\xi\eta}$ in the given iteration of solution of (*1*), (*2*). These equations may be in general of the form

$$-x_\xi + \varphi_{\xi\chi}\sum_\eta x_\eta = 0 \tag{48}$$

but can be transferred in the form (*47*) by introduction of a fictive variable x_χ and the additive equation:

$$-x_\chi + \sum_\eta x_\eta = 0\,. \tag{49}$$

In a technological schema, the equation (*49*) is the model of a fictive mixing node. For further considerations in this part, we take the set $\{\eta\}$ as the set of subscripts of those variables x, which are multiplied in some equation of the subset (1) by a parameter $\varphi_{\xi\eta}$.

For the solution of the set (1), (2), including the equations (*47*) and (*49*), we construct the matrix of coefficients of the linear subset (1) $\mathbf{A}$ in the way that we ignore the parameters φ as non-zero coefficients and express their occurrence in (1) by a matrix $\mathbf{B}(M, N) = (\bar{b}_{ij})$, where

$$\bar{b}_{ij} = \begin{cases} 1 & \text{in case of multiplying the variable } x_r \text{ in the } i\text{-th equation of } (1) \text{ by the} \\ & \text{parameter } \varphi_{jr} \\ 0 & \text{otherwise} \end{cases}$$

At the same time, we give up the matrix of parameters $\Phi(N, N) = (\varphi_{rj})$. The equation (3) is now of the form:

$$(\mathbf{A} + \bar{\mathbf{B}}\Phi)\,\mathbf{X} + \mathbf{C} = \mathbf{O} \tag{50}$$

and the occurrence matrix $\mathbf{B}$ is constructed from the information, contained in $\mathbf{A}$, in the way that

$$b_{ij} = \begin{cases} 1 & \text{for } (a_{ij} \neq 0) \cap (\varphi_{(r)j} = 0) \\ 0 & \text{otherwise} \end{cases}$$

and the starting values of β_j, γ_j in Step A. of Algorithm 1. are determined as

$$\beta_j = \gamma_j = \begin{cases} 1 & \text{if } b_{(i)j} = 0 \text{ or } \sum_r \varphi_{rj} \neq 0,\ \{r\} \leftrightarrow \{j\}. \\ 0 & \text{otherwise} \end{cases}$$

With respect to (8), the equation (50) may be expressed as

$$\mathbf{U}(\mathbf{A} + \bar{\mathbf{B}}\Phi)(\mathbf{V}_E\mathbf{Y}_E + \mathbf{V}_R\mathbf{Y}_R) + \mathbf{UC} = \mathbf{O}. \tag{51}$$

The way of construction of the matrices $\mathbf{A}$ and $\mathbf{B}$ indicates that the variables x_ξ from the relation (47) are always among the eliminated variables and the variables x_η among the remaining variables, so that

$$x_\xi = \varphi_{\xi\eta} x_\eta . \tag{52}$$

It is caused by the fact that in equations (47) may be as output variables determined only the variables x_ξ. Otherwise the degeneracy of the linear subset (1) may occur, *i.e.* the number of variables, which can be determined through (1), is less than M. It would happen only in cases, where

a) there is besides the equation (47) an equation

$$a_{m\xi} x_\xi + a_{m\eta} x_\eta + c_m = 0 \tag{53}$$

in (1), or

b) the equations

$$-x_{\xi_1} + \varphi_{\xi_1\eta_1} x_{\eta_1} = 0 \tag{54}$$

$$-x_{\eta_1} + \varphi_{\eta_1\eta_2} x_{\eta_2} = 0 \tag{55}$$

simultaneously occur in (1).

The occurrence of both cases is of no sense, however. In the case ad *a*), with regard to the exclusive common occurrence of the variables x_ξ and x_η in equations (*47*) and (*53*) the latter equation must be a part of the rigorous model represented by the parameter $\varphi_{\xi\eta}$ and cannot therefore be an equation of the subset (1). In the case ad *b*), it is useful to combine both equations (*54*), (*55*) (and both representative models, too) with the result

$$-x_{\xi_1} + \varphi_{\xi_1\eta_2} x_{\eta_2} = 0\,, \tag{56}$$

where $\varphi_{\xi_1\eta_2} = \varphi_{\xi_1\eta_1}\varphi_{\eta_1\eta_2}$. Thus

$$\bar{\mathbf{B}}\Phi\mathbf{V}_E = \mathbf{O} \tag{57}$$

and

$$\mathbf{Y}_E = -\left[(\mathbf{A}_U + \mathbf{A}_U^\Phi)\,\mathbf{Y}_R + \mathbf{C}_U\right], \tag{58}$$

where

$$\mathbf{A}_U^\Phi(M, N - M) = \bar{\mathbf{A}}_U\Phi\mathbf{V}_R \tag{59}$$

$$\bar{\mathbf{A}}_U(M, N) = (\bar{a}_{ij}^U) = (\mathbf{U}\mathbf{A}\mathbf{V}_E)^{-1}\,\mathbf{U}\bar{\mathbf{B}}\,. \tag{60}$$

The relation

$$\mathbf{X} = -\left[(\mathbf{A}_V + \mathbf{A}_V^\Phi)\,\mathbf{Y}_R + \mathbf{C}_V\right] \tag{61}$$

is analogous to the relation (*13*) and

$$\mathbf{A}_V^\Phi(N, N - M) = (a_{jk}^{V\Phi}) = \mathbf{V}_E\mathbf{A}_U^\Phi\,. \tag{62}$$

The matrix $\mathbf{W}(N, N - M) = (w_{jk})$ is now constructed as

$$w_{jk} = \begin{cases} 1 & \text{for } (a_{jk}^V \neq 0) \cup (a_{jk}^{V\Phi} \neq 0)\,. \\ 0 & \text{otherwise} \end{cases}$$

Thus, due to the formulation of the equation (*3*) in the form of (*50*), the repetitive correction of parameters φ is connected with the solution of the nonlinear set (2). The correction of φ's concerns only those matrices, which do depend on them, *i.e.* the matrices $\mathbf{A}_U^\Phi$ and $\mathbf{A}_V^\Phi$. The reduced occurrence matrix $\mathbf{Q}_R$ is given by the formula (*16*) again. The relation:

$$\mathbf{X} = -\left[(\mathbf{H}_I + \mathbf{H}_I^\Phi)\,\mathbf{Z}_I + (\mathbf{H}_C + \mathbf{H}_C^\Phi)\,\mathbf{Z}_C + \mathbf{C}_V\right] = -\left[(\mathbf{H} + \mathbf{H}^\Phi)\,\mathbf{Z} + \mathbf{C}_V\right], \tag{63}$$

where for the matrices $\mathbf{H}_I^\Phi(N, L - M)$, $\mathbf{H}_C^\Phi(N, N - L)$ and $\mathbf{H}^\Phi(N, N - M)$ the relation

$$(\mathbf{H}_I^\Phi, \mathbf{H}_C^\Phi) = (\mathbf{A}_V^\Phi\mathbf{D}_I, \mathbf{A}_V^\Phi\mathbf{D}_C) = \mathbf{A}_V^\Phi\mathbf{D} = \mathbf{H}^\Phi = (h_{jk}^\Phi) \tag{64}$$

is valid, is analogous to the relation (*24*). It is necessary to add the matrices $\mathbf{V}$, $\mathbf{D}$, $\bar{\mathbf{A}}_U$, Φ, $\mathbf{A}_V^\Phi$ and $\mathbf{H}^\Phi$ to those mentioned above, the elements of Φ, $\mathbf{A}_V^\Phi$ and $\mathbf{H}^\Phi$ change their values during the solution of (2). It is mostly the question of physical character of x_η, whether this variable is to be considered as the iterated variable or the control one.

We may resolve the problem just before starting with Algorithm 2 or state role of x's at the very beginning of the computation. From the general point, the role of these variables is for any technique of solution of sets of algebraic equations irrelevant but it is of great importance when a real physical process is to be analyzed. Moreover, it is not the same thing to correct the φ's in any iteration of the solution of the subset (2) or in connection with any change in the values of control variables (*e.g.* for needs of an optimization procedure). It is not the purpose of this paper, however, to make a manysided analysis of the problem, all we are interested in is how to situate the individual x_η's among the elements of $\mathbf{Z}$.

If we wish to have the variables x_η among the iterated ones, we state in Step A of Algorithm 2 the quantities

$$\vartheta_j = \begin{cases} 0 & \text{for } a_{\{k\}j}^{V\Phi} = 0\,; \quad \{k\} \leftrightarrow k = 1, \ldots, N \\ 1 & \text{otherwise} \end{cases}$$

$$\alpha_i = \begin{cases} 1 & \text{for } \sum_j (1 - \vartheta_j)\, q_{ij}^R = 0 \\ 0 & \text{otherwise} \end{cases}$$

and in Step F an additive condition

$$\alpha_i = \begin{cases} 1 & \text{for } \sum_n (1 - \vartheta_n)\, q_{in}^R = 0 \\ 0 & \text{otherwise} \end{cases}$$

and the set of subscripts $\eta(s)$ in a changed form

$$\{\eta(s)\} \leftrightarrow \{j \mid (q_{sj}^R = 1) \cap (\beta_j = 0) \cap (\vartheta_j = 0)\}$$

(If now $\alpha_s = 1$ for all s's we return to the Step C, otherwise we continue with those s's, for which $\alpha_s = 0$). The other instructions of Algorithm 2 remain unchanged.

If we wish, on the contrary, to have the x_η's among the control variables, the quantities β and γ get in Step A of Algorithm 2 the values

$$\beta_k = \gamma_k = \begin{cases} 1 & \text{if } \vartheta_j^R = 1 \quad \text{or} \quad \sum_j a_{jk}^{V\Phi} \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

Algorithm 2. can be adapted in a similar way for any other conditions concerning the variables x_η. In both mentioned cases, it cannot be forgotten that the "free" space for the determination of x_η's, as iterated or control variables, is given by the quantity $(N - L)$ minus the number of preliminary selected control variables. According to the "pure" coordination of x_η's to iterated or control variables, the matrices $\mathbf{H}_I$ or $\mathbf{H}_C$ in the relation (63) are zero matrices.

For the identification of the occurrence of the variables x_η in individual subsystems of equations (or control variables vector), a Boolean vector $\omega(N - M, 1) = (\omega_j)$ with the help of the vector $\vartheta = (\vartheta_j)$ and the relation:

$$\omega = \mathbf{D}^T\vartheta \qquad (65a$$

is constructed. In common with it the sets of subscripts

$$\left.\begin{array}{l} j = 1, \ldots, N \\ n, r = M + 1, \ldots, N \\ \{l\} \leftrightarrow \{n \mid \omega_n = 1\} \\ \{k\} \leftrightarrow \{j \mid v^R_{jr} d_{r1} = 1\} \\ \{i\} \leftrightarrow \{j \mid \varphi_{jk} \neq 0\} \end{array}\right\} \qquad (A)$$

are set up. According to Algorithm 3, after the solution of s'th subsystem for given values of φ's (Step G), the values of the parameters φ_{ik} are corrected by the solution of consistent rigorous models. For the corrected values of φ's, the Step G is repeated as long as the changes in successive values of φ's exceed the prescribed tolerance. The given subsystem is considered to be resolved if the desired accuracy level is reached for $z_{\{n\}}$ and for $\varphi_{i\{k\}}$ as well. It is apparent that for particular x_η as a control variable the consistent φ's are corrected simultaneously with any change in the value of x_η.

Practical Aspects of the Computational Algorithm

When deriving the relations between the eliminated and remaining variables and further the iterated and the control ones we have strictly followed for the sake of clearness and homogenity of expressions the matrix and vector form of the presented formulas. From the point of computation, this way of expressions has a drawback – the solution of extensive problems paralyses a good deal of computer storage. It is the purpose of this part to show how it is possible to lower the requirements on computer storage.

Certain succes may be achieved by the direct replacing of the matrices $\mathbf{U}$, $\mathbf{V}$ by the vectors α and $\gamma\,(= \gamma^1)$ from Steps G-J of Algorithm 1. From the way of construction

of the matrix **U** follows for the matrix products $\mathbf{UA} = \mathbf{A}'$, $\mathbf{U\bar{B}} = \bar{\mathbf{B}}'$ and $\mathbf{U\bar{C}} = \bar{\mathbf{C}}'$ that the m-th rows of original matrices **A**, $\bar{\mathbf{B}}$ and **C** become i-th rows of the row-reorganized matrices $\mathbf{A}'$, $\bar{\mathbf{B}}'$ and $\mathbf{C}'$ if $\gamma_{\alpha_m} = i$. Similarly, for the column-reorganized matrices $\mathbf{A}'$ and Φ (*i.e.* $\mathbf{A}''$ and Φ'), the condition $\gamma_n = j$ implies that the m-th columns of $\mathbf{A}'$ and Φ become j-th columns of $\mathbf{A}''$ and Φ'. Thus the multiplication by **U** from left and **V** from right is replaced by the implication

$$(\gamma_k = i, \alpha_m = k, \gamma_n = j) \Rightarrow a''_{ij} = a_{mn}\,, \quad \bar{b}'_{ij} = \bar{b}_{mj}\,, \quad \varphi'_{rj} = \varphi_{rn}\,,$$
$$c'_i = c_m\,, \quad \vartheta^R_j = \vartheta_n (j > M)\,. \tag{65b}$$

The starting approximations of values of the parameters φ are considered non-zero (and according to their very existence, non-zero values may be adjusted on them through the whole solution). Let us denote formally the first M columns of $\mathbf{A}''$ as a matrix $\mathbf{A}''_1$, the other $N - M$ columns of $\mathbf{A}''$ as a matrix $\mathbf{A}''_2$ and the last $N - M$ columns of Φ' as a matrix Φ'_2*) – then the relations (*11*), (*12*), (*59*)–(*60*) may be written as:

$$\mathbf{A}_U = (\mathbf{A}''_1)^{-1}\,\mathbf{A}''_2 \tag{66}$$

$$\bar{\mathbf{A}}_U = (\mathbf{A}''_1)^{-1}\,\bar{\mathbf{B}}' \tag{67}$$

$$\mathbf{A}^{\Phi}_U = \bar{\mathbf{A}}_U \Phi'_2 \tag{68}$$

$$\mathbf{C}_U = (\mathbf{A}''_1)^{-1}\,\mathbf{C}'\,. \tag{69}$$

For the numeration of the matrices $\mathbf{A}_V$, $\mathbf{A}^{\Phi}_V$ and the vector $\mathbf{C}_V$ serves the implication

$$(\gamma_j = n) \Rightarrow a^V_{jk} = \begin{cases} a^U_{nk} & \text{for} \quad n \leqq M \\ -1 & \text{for} \quad k = n > M \\ 0 & \text{otherwise} \end{cases}, \quad a^{V\Phi}_{jk} = \begin{cases} a^{U\Phi}_{nk} & \text{for} \quad n \leqq M\,, \\ 0 & \text{otherwise} \end{cases}$$

$$c^V_j = \begin{cases} c^U_n & \text{for} \quad n \leqq M\,. \\ 0 & \text{otherwise} \end{cases} \tag{70}$$

It is apparent that the constraints (*28*) are transformed on the remaining variables according to the implication

$$(\gamma_j = n > M) \Rightarrow y^L_n,\, y^U_n = x^L_j,\, x^U_j\,. \tag{71}$$

* With regard to the simple transformation $\Phi \leftrightarrow \Phi'$ the matrix Φ' is not necessary at all It is presented here only for the sake of convenience.

The reduced occurrence matrix $\mathbf{Q}_R$ may be constructed without using the matrix $\mathbf{W}$, the values of its elements are given by the relation

$$q^R_{ik} = \begin{cases} 1 & \text{for } \sum_j q_{ij}\left(\left|a^V_{jk}\right| + \left|a^{V\Phi}_{jk}\right|\right) \neq 0 \,. \\ 0 & \text{otherwise} \end{cases} \tag{72}$$

Similarly, we can replace the matrices $\mathbf{D}$ and $\mathbf{E}$ by the vectors α and γ $(= \gamma^2)$ from Steps G-J of Algorithm 2. The elements of the occurrence matrix $\mathbf{Q}_I$ are given by

$$(\gamma_k = j \leqq L) \Rightarrow q^I_{ij} = q^R_{ik} \tag{73}$$

and the elements of the adjacency matrix $\mathbf{P}$ are given by the condition for replacement of the m-th row of $\mathbf{P}$ by j-th column of $\mathbf{Q}_I$ if $\gamma_{\alpha_m} = j$, or

$$(\gamma_k = j,\ \alpha_m = k) \Rightarrow p_{mi} = q^I_{ij} \,. \tag{74}$$

Both relations (*73*), (*74*) may be united in the form

$$(\gamma_k = j \leqq L\,,\ \alpha_m = k) \Rightarrow p_{mi} = q^R_{ik} \tag{75}$$

which enables to exclude the matrix $\mathbf{Q}_I$ from our considerations. The transformation of the variables z on the variables x is given by the relation (*23*), where the matrices $\mathbf{H}$ and $\mathbf{H}^\Phi$ are constructed according to the relation:

$$(\gamma_k = n) \Rightarrow h_{jn} = a^V_{jk}\,,\ h^\Phi_{jn} = a^{V\Phi}_{jk} \,. \tag{76}$$

Let us remind that z_j $(j = M + 1, \ldots, L)$ are the iterated variables for which the subset of nonlinear equations (*2*) is solved and z_k $(k = L + 1, \ldots, N)$ are the control variables, the knowledge of particular values of which is for the solution of (*2*) on given iteration step unavoidable. The constrains (*28*) are on these variables transformed by the relation (*75*) and

$$(\gamma_n = k) \Rightarrow z^L_k,\ z^U_k = y^L_n,\ y^U_n \,. \tag{77}$$

Knowing the vector γ^2 and the matrices $\mathbf{Q}_R$, $\hat{\mathbf{G}}$, we can construct the matrix of variables of individual subsystems of equations $\mathbf{T}$ without using the matrix $\mathbf{Q}_I$ following the succession of instructions

$$s = 1, \ldots, S$$

$$k = M + 1, \ldots, L$$

$$j = M + 1, \ldots, N$$

$$\{m\} \leftrightarrow \{j \mid \gamma_j \leqq L\}$$

$$t_{s\gamma m} = \sum_k B g_{sk} q^R_{km} .$$

The vector ω, which indicates the occurrence of the variables x_n in individual subsystems (or in the vector of control variables), is related to the vector $\bar{\vartheta}$ from Algorithm 2 by

$$(\gamma_n = k) \Rightarrow \omega_k = \bar{\vartheta}_n \tag{78}$$

and the set of subscripts (A) is now of the form

$$\left.\begin{array}{l} j = 1, \ldots, N \\ n, r = M + 1, \ldots, N \\ \{l\} \leftrightarrow \{n \mid \omega_n = 1\} \\ \{k\} \leftrightarrow \{j \mid (\gamma^1_j = r) \cap (\gamma^2_r = l)\} \\ \{i\} \leftrightarrow \{j \mid \varphi_{jk} \neq 0\} \end{array}\right\} \tag{A'}$$

The relation

$$(\gamma^1_j = n) \Rightarrow a^{V\Phi}_{jk} = \begin{cases} \sum_{m=1}^{N} \bar{a}^U_{nm} \varphi'_{mk} & \text{for} \quad n \leqq M \\ 0 \quad \text{otherwise} \end{cases} \tag{79}$$

is used in Algorithm 4. for the correction of $\mathbf{A}^{\Phi}_{V}$ and $\mathbf{H}^{\Phi}$ due to changes in values of φ's.

Not all the matrices and vectors mentioned in this part must be necessarily stored in computer memory throughout the whole computation. Table I presents the position of individual matrices and vectors, used during computation, in the required field of dimension $N \times (7N + 14)$ (from which the part of $4(N \times N)$ is occupied due to the existence of the parameters φ). Together with those of other algorithms, necessary for the simulation of complex processes as a whole, these requirements put the restrictions on practical utilization of the presented global approach with respect to the extent of a particular problem and to the possibilities of a given computing technique. As for the solution of sets of nonlinear algebraic equations itself, the other necessary matrices and vectors (Jacobian, its inverse *etc.*) are not included in the mentioned field.

TABLE I

The Position of Matrices and Vectors in the Field of N Rows during Computation

Type of Matrix	Real										Integer								
No of Columns	N	N	N	N	N	1	1	1	1	1	N	N	1	1	1	1	1	1	1
Data	$\mathbf{A}$		$\mathbf{\Phi}$			$\mathbf{X}$	$\mathbf{X}_U$	$\mathbf{X}_L$		$\mathbf{C}$	$\mathbf{B}$	$\overline{\mathbf{B}}$							ϑ
Algorithm 1												$\overline{\mathbf{Q}}$	γ^1		α	β	θ/ψ	η	
$\mathbf{A}''$, $\mathbf{B}'$, $\mathbf{C}'$, $\mathbf{Y}_L$, ϑ_R			$\mathbf{A}''$					$\mathbf{Y}_L$	$\mathbf{C}'$			$\overline{\mathbf{B}'}$							
$\mathbf{Y}_U$, $(\mathbf{A}_1'')^{-1}$	$(\mathbf{A}_1'')^{-1}$									$\mathbf{Y}_U$		$\overline{\mathbf{Q}}$	ϑ_R						
$\mathbf{A}_U$, $\mathbf{C}_U$	$(\mathbf{A}_1'')^{-1}$, $\mathbf{A}_U$						$\mathbf{C}_U$												
$\overline{\mathbf{A}}_U$			$\overline{\mathbf{A}}_U$									$\overline{\mathbf{Q}}$							
$\mathbf{A}_U^{\Phi}$		$\mathbf{A}_U^{\Phi}$																	
$\mathbf{A}_V^{\Phi}$, $\mathbf{C}_V$				$\mathbf{A}_V^{\Phi}$					$\mathbf{C}_V$										
$\mathbf{A}_V$		$\mathbf{A}_V$																	
$\mathbf{Q}_R$											$\mathbf{Q}_R$								
Algorithm 2														γ^2	α	β	θ/ψ	η	$\overline{\vartheta}$
$\mathbf{p}^{(k)}$, $\mathbf{p}^{(2k)}$											$\mathbf{p}^{(2k)}$	$\mathbf{p}^{(k)}$							
$\mathbf{Z}_L$, $\mathbf{H}$, $\mathbf{G}$ (Alg. 3)	$\mathbf{H}$						$\mathbf{Z}_L$					$\mathbf{G}$							
$\mathbf{Z}_U$, $\mathbf{H}^{\Phi}$, $\hat{\mathbf{G}}$		$\mathbf{H}^{\Phi}$						$\mathbf{Z}_U$			$\hat{\mathbf{G}}$								
$\mathbf{T}$, ω												$\mathbf{T}$	ω						
$\mathbf{F}^a$, Alg. 4	$\mathbf{H}$	$\mathbf{H}^{\Phi}$	$\mathbf{\Phi}$	$\mathbf{A}_U$	$\mathbf{A}_V^{\Phi}$	$\mathbf{X}$	$\mathbf{Z}_L$	$\mathbf{Z}$	$\mathbf{Z}_U$	$\mathbf{C}_V$	$\mathbf{F}$	$\hat{\mathbf{G}}$	$\mathbf{T}$	ω	γ^1	γ^2	α	β	

[a] $\mathbf{F} \equiv \mathbf{F}(\mathbf{X}) = (f_k(\mathbf{X}))$; $k = M+1, \ldots L$

CONCLUSION

The described method of global approach to the steady state simultation of complex technological processes considers the solution of mixed ((*i.e.* linear and nonlinear) sets of algebraic equations of the mathematical model of a system in a single computational block. The method is quite general, the solution of submodels with special computational algorithms is respected by the intercession of their representative models. This point bears some features of the sequential approach to the simulation and is simple enough to unite the distinctive elements of both approaches if necessary. Presented paper doesn't pretend to discuss the problem of representative models exhaustively, much remains to be done for their stability and convergence evaluation. According to the knowledge and experience gained so far it may be assumed that the proposed way of their utilization is general enough.

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