# SIMPLE ALGORITHM OF DECOMPOSITION OF EQUATIONAL MODELS OF GLOBAL SIMULATION OF COMPLEX SYSTEMS

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Simple algorithm is described for decomposition of equational sets forming mathematical models of complex chemical-process systems at their global simulation in unsteady state. The algorithm does not require calculation of powers of adjacent matrix as is usual with the currently used methods based on the theory of graphs. The needed numerical operations are performed on the given matrix of occurrence of variables in individual equations of the system only.

Possible decomposition of models of complex systems is one of significant features of progressive approach to the solution of their simulation problems. It contributes first of all to speeding and higher possible accuracy of solution, with complex problems it is sometimes the way how to obtain calculation convergence. The usual methods of decomposition of equation sets based on the theory of graphs lead directly to determination of possible, in some hierarchy independently solvable subsystems. They are mathematically elegant, formally simple and easily programmable. The disadvantage is their greater stress on computer memory and neccesity of additional comparison of decomposition results with the structure of the set of equations for determination of the sequence of solution of individual subsystems.

Mathematically, the equational model of a simulated complex system in steady state is represented by a system of $L$ algebraic equations with $N$ variables

$$f_i(\boldsymbol{X}) = f_i(x_1, \ldots, x_N) = 0\,; \quad i = 1, \ldots, M, \; M + 1, \ldots, L \leqq N\,. \qquad (1)$$

Let us assume that the first $M$ equations of the system (without affecting generality are linear, *i.e.*

$$f_i(\boldsymbol{X}) = \sum_{j=1}^{N} a_{ij} x_j + c_i = 0\,; \quad i = 1, \ldots, M\,. \qquad (2)$$

Moreover let us assume that the system as regards the number of explicit variables in individual equations is sufficiently sparse (certain sparsity of the system is actually the necessary condition of the possibility of its decomposition). But this assumption

is stated with full agreement with the typical structure of any model of complex chemical-technology system.

In general, for the system of $n$ equations with $n$ variables, when it is consistent and definite (*i.e.* when it is solvable according to its variables and the number of solutions is finite) there holds that any subsystem of equations with $m_k$ variables cannot include more than $n_k$ equations of the system:

*1*) When the subsystem with $n_k$ variables is formed by $n_k$ equations of the system, it is then consistent and definite. Definity of subsystem is here given by the number of equations and variables. It consistency then preconditions the assumed consistency of the whole system.

*2*) If the subsystem of $n_k$ variables is formed by $m_k$ equations of the system, while $m_k > n_k$, then information contained in any arbitrary $(m_k - n_k)$ equation of this system is for its solvability excessive and on the contrary necessarily must be lacking in the subsystem formed by the remaining $(n - m_k)$ system equations. But in this case the system cannot be consistent which is in contradiction with the initial assumption.

*3*) In the case $m_k < n_k$ consistency of the subsystems is not disturbed. It is always possible to find for $(n_k - m_k)$ of suitably selected variables such values that the subsystem becomes moreover also definite. These values must necessarily exist due to the initial assumption.

It directly results that to each equation of a consistent system can be mutually uniquely adjoined an output variable, *i.e.* the variable whose value can be from given values of other explicit variables calculated by use of the given equation. When the system is definite the output variables of all equations form a closed continuous chain of information flow among individual equations. Existence of this chain is the precondition of existence of solution of the given system of equations. Impossibility of finding the complete vector of output variables necessarily and at the same time sufficiently indicates inconsistency of the solved system of equations which means that the simulation problem is wrongly formulated.

In general case the selection of output variables for the given system does not need to be unique. This ambiguity does not cause any additional problems as regards decomposition of the system of equations in the case of simple simulation. It can only become a problem in solution of individual subsystems by use of some of the methods of direct substitution. But with optimal simulation* the ambiguity in selec-

* The term optimal simulation is used here in the sense of selection of such values of control variables which lead to determination of the minimal (maximal) value of an objective function in the area of feasible solutions. As concerns the technique of selection of variables for control purposes or simple solution of the system on required level of its control included here is also the case of selection of some of variables as a parameter whose value is in advance determined and already not changed during the solution of the simulation problem.

tion of output variables can be effectively utilized for maximum decomposition of the system and thus also for maximum decrease of its dimension.

This possibility has been for example studied by Ramirez and Vestal[1].

The effect of selection of output variables to the level of decomposition of the system can be illustrated by a simple example: Let us consider optimal solution of the simulation problem modelled by four equations with five variables

$$f_1(x_1, x_3) = 0 \tag{3a}$$

$$f_2(x_1, x_3, x_4) = 0 \tag{3b}$$

$$f_3(x_1, x_2, x_4) = 0 \tag{3c}$$

$$f_4(x_2, x_3, x_4, x_5) = 0\,. \tag{3d}$$

The system thus has one degree of freedom which can be used for optimisation of functioning of the system. Possible selection of control variable with a corresponding level of decomposition of the system are these:

$$x_1\colon\ f_1 \xrightarrow{x_3} f_2 \xrightarrow{x_4} f_3 \xrightarrow{x_2} f_4 \xrightarrow{x_5}$$

$$x_2\colon\ \left.\begin{matrix} f_1 \\ f_2 \\ f_3 \end{matrix}\right\} \xrightarrow{x_1, x_3, x_4} f_4 \xrightarrow{x_5}$$

$$x_3\colon\ f_1 \xrightarrow{x_1} f_2 \xrightarrow{x_4} f_3 \xrightarrow{x_2} f_4 \xrightarrow{x_5}$$

$$x_4\colon\ \left.\begin{matrix} f_1 \\ f_2 \end{matrix}\right\} \xrightarrow{x_1, x_3} f_3 \xrightarrow{x_2} f_4 \xrightarrow{x_5}$$

$$x_5\colon\ \left.\begin{matrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{matrix}\right\} \xrightarrow{x_1, x_2, x_3, x_4}$$

Maximum level of decomposition is reached by selection of variable $x_1$ or $x_3$ as the control variable, selection of variable $x_5$ on the other hand enables no decomposition at all.

The aim of this study is to describe an algorithm of selection of variables and decomposition of the system for determination of optimal vector of output variables by use of the modified method published earlier by the author[2]. By determination of output variables of linear equations of the system (if they exist) is reached the first degree of decomposition – is obtained solution of the subsystem of linear

equations according to their output variables (so-called eliminated variables) in dependence on output variables of the subsystem of nonlinear equations (so-called iterated variables) and control variables (or system parameters). Iterated and control variables are then the proper subject of solution of the simulation problem[2]. In the case the model of simulated system is formed by linear equations only, the solution of the model for the given control level is obtained in the first stage of decomposition.

Modification of the mentioned method of determination of output variables is closely related with the proposed method of decomposition of nonlinear subsystem. This heuristic method has minimal requirements on the computer memory as it operates only on the matrix of occurrence of variables and a small number of auxiliary vectors. The occurrence matrix $\mathbf{Q} = (q_{ij})$ is the Boolean matrix with unit value of element $q_{ij}$ only in the case when the variable $x_j$ is the explicit variable of equation $f_i$). The result of decomposition *i.e.* factorization of the system of equations into individual subsystems and sequence of their solution is obtained at once in a concise form of at most three vectors with the maximum dimension $N$. The method is simple and easily programmable. Total number of instructions in comparison with the methods based on the graph theory is by about one third smaller.

The whole algorithm of decomposition of equational set, determination of eliminated, iterated and control variables can be described by these steps:

*Determination of Output Variables*

This step has an imminent significance for the solution of the subsystem of linear equations where the output variables are at the same time the eliminated variables. By determination of output variables of the subsystem of nonlinear equations the possible degeneration of subsystems is prevented, which is due to unsuitable selection of control variables (when these are not fixed in advance). With the optimisation problems (*i.e.* $L < N$) the selection of control variables gives a chance for a maximum decomposition of the system.

Step A. $\{i\} \leftrightarrow i = 1, \ldots, L$

$\{j\} \leftrightarrow = 1, \ldots, N$

$\alpha_{\{i\}} = 0,\ \beta_{\{j\}} = 0,\ \gamma_{\{j\}}$ given

When $(\tau = 0) \cap (\pi = 2)$, continue by Step G.

The quantities $\alpha_i$ and $\beta_j$ serve for indication of the selected $x_j$ as output variable of equation $f_i(\mathbf{X}) = 0$, *i.e.* $\alpha_i = j$ and $\beta_j = 1$; otherwise $\alpha_i = 0$ and $\beta_j = 0$. Possibility or impossibility to obtain the complete vector of output variables indicates also the formal correctness or incorrectness of formulation of the simulation problem.

The requirement of the role of control variable for $x_j$ is given by the value $\gamma_j = 1$ (otherwise $\gamma_j = 0$, the control variable cannot be simultaneously the output variable). For simple simulation ($L = N$) there holds $\tau = 0$, while for optimal (controlled) simulation ($L < N$) there holds $\tau = 1$. Moreover there holds $\pi = 1$ – system is formed only by linear equations ($L = M$); $\pi = 2$ – system is formed only by nonlinear equations ($M = 0$); $\pi = 3$ – system form both linear as well as nonlinear equations ($M < L$). In this case combination $(\tau = 0) \cap (\pi = 2)$ means that in the case of simple simulation on the system of nonlinear equations the question of output variables is not of interest and algorithm continues directly by the verification of the possibility of system decomposition.

Step B. If $\alpha_{\{i\}} \neq 0$, continue by Step E.

Fulfilment of the requirement $\alpha_i \neq 0$ for all $i$ means that the output variable of each equation of the system is determined and algorithm can continue by eventual notation of control variables and by solution of the linear subsystem or by possible decomposition of nonlinear subsystems.

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

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

$\Theta_m = \sum_n q_{mn}$

$\{r\} \subset \{m\}\colon\ \Theta_r = \min_m [\Theta_m]$

If $\Theta_r > 1$, continue by Step D.

Otherwise let $\Theta_r = q_{rs} = 1\ (s \in \{n\})$, then $s \to \alpha_r$, $1 \to \beta_s$.

Return back to Step B.

With equations which do not have their output variable yet determined is of interest the number of variables which are neither control nor output variables (for other equations of the system). They are obtained by row summations of the occurrence matrix $\Theta_m$. When in some equation (or equations) is only one such variable (*i.e.* $\Theta_r = 1$), it must necessarily be the output variable (variables) for this equation (equations). Neglect of equation with one single variable which could so become the output variable of another equation (and also of an equation with even several variables) leads to degeneration of the system as not all equations then have their output variables. It is obvious that at correctly formulated problem, when the occurrence matrix **Q** has the maximum rank $L$, there always holds $\Theta_m \geqq 1$ for all $m$.

Step D. $\varepsilon_n = \sum_m q_{mn}$

$\{t\} \subset \{n\} : \varepsilon_t = \min_n [\varepsilon_n | \varepsilon_n > 0]$

for all $t$: $\{\xi_t\} \leftrightarrow \{m | q_{mt} = 1\}$

$\psi_t = \sum_n \sum_{\xi_t} \mathrm{B}\, q_{\xi_t n} - \varepsilon_t$

($\sum \mathrm{B}$ – symbol of the Boolean summation)

$\{s\} \subset \{t\} : \psi_s = \min_t [\psi_t]$

For an arbitrary $s$: $\{r\} \subset \{\zeta_{sj}\} : \Theta_r = \min_{\xi_s} [\Theta_{\xi_s}]$

For an arbitrary $r$: $s \to \alpha_r$, $1 \to \beta_s$.

Return back to Step B.

When the occurrence of variable $x_s$ in all equations $f_m(x_{(n)}) = 0$ is minimal ($\varepsilon_t$), the incidence between the equation $f_r(\mathbf{X}) = 0$ for which $x_s$ is the output variable and other equations of the system is then also minimal. In consequence it is possible to reach higher degrees of decomposition of the system. The quantity $\psi_t$ denotes the number of degrees of freedom of variable $x_t$ defined as total number of variables in equations which include $x_t$, reduced for the number of these equations (actually there suffices to determine within $\psi_t$ only the number of variables *i.e.* the first term of the relation for $\psi_t$ as the column sum of $\varepsilon_t$ is for all $x_t$ identical). The greater is the degree of freedom (*e.g.* of the variable $x_k$) the greater is the number of equations which otherwise do not include $x_k$ and which must be added to equations with explicite occurrence of $x_k$ so that a subsystem with maximal (*i.e.* full) rank would be formed. This results in reduction of the accessible degree of system decomposition. Condition $\varepsilon_n > 0$ at selection of $\varepsilon_t$ is due to inequality $L < N$ in case of optimal simulation. Smaller number of equations than variables admits possible "vanishing" of some variables with equations for which the degrees of freedom were already determined.

*Notation of Control Variables*

This phase is the natural result of selection of output variables at $\tau = 1$ (*i.e.* $L < N$). Variables which were not selected as output variables must take the task of control variables or system parameters with given constant values when the optimisation problem is not concerned (in this case the quantity $\tau$ becomes equal to 0.)

Step E. If $\tau = 0$, continue by Step F.

$\{n\} \leftrightarrow \{j | \beta_j = 0\}$

$\gamma_{(n)} = 1$

If $\pi = 2$, continue by Step G.

*Solution of Subsystem of Linear Equations*

By expressing the dependence of eliminated variables $x_{\alpha_m | m \leqq M}$ on the iterated and control ones ends the first phase of decomposition, reducing the original system of dimension $L \times N$ to the system of dimension $(L - M) \times (N - M)$, or $(L - M) \times (L - M)$ when the elimination of control variables is considered at the same time. The constants $c'$ and coefficients $a'$ are in a general expression of the mentioned dependence an inversion image of original constant $c$ and of coefficients $a$ at the noneliminated variables.

Step F. $\{m\} \leftrightarrow \{i | i \leqq M\}$

$\{n\} \leftrightarrow \{j | j \notin \{\alpha_m\}\}$

$x_{\alpha_m} = c'_m + \sum_n a'_{mn} x_n$

If $\pi = 1$, STOP.

$\{i\} \leftrightarrow i = M + 1, \ldots, L$

$\{k\} \leftrightarrow \{j\}$

$$q_{ik} = \begin{cases} 1 & \text{if} \quad (k = \alpha_l | \, l > M) \cap (q_{ik} = 1) \\ & \text{or} \quad (q_{ij} = 1) \cap (j = \alpha_l | \, l \leqq M) \cap (a'_{ik} \neq 0) \\ 0 & \text{otherwise} \end{cases}$$

When the system is formed by only linear equations then by calculation of the simulation problem this phase practically ends (at least for the given control). Otherwise it is necessary to project the made elimination of variables and reduction of the system into the occurrence matrix **Q**.

Step G. $\vartheta_{(i)} = 0$, $\eta_{(j)} = 0$

$$\beta_j = \begin{cases} 1 & \text{If} (\gamma_j = 1) \text{ or } (j = \alpha_l | \, l \leqq M) \\ 0 & \text{otherwise} \end{cases}$$

$0 \rightarrow \omega$

*Decomposition of Subsystem of Nonlinear Equations*

The aim of decomposition is to find in the system of equations a relatively independently soluble subsystems and to determine the hierarchy of sequence of their solubility with regard to the knowledge of values of their explicite variables. Decomposition thus enables further reduction of the system size. Sequence of solubility is determined by increasing value of quantity $\omega$, $\omega = 1, \ldots, \Omega$, where $\Omega$ is the number of found subsystems. Relationship of the $i$-th equation or of $j$-th variable to the $\omega$-th subsystem is indicated by quantities $\vartheta_i = \omega$ or $\eta_j = \omega$.

Step H. If $\vartheta_{\{i\}} \neq 0, \omega \to \Omega$, STOP.

$\{m\} \leftrightarrow \{i \mid \vartheta_i = 0\}$

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

$\omega + 1 \to \omega$

$\{s\} \subset \{m\}$: in this point $\{s\}$ is an empty set of indices from $\{m\}$

The set of indices $\{s\}$ includes in general the indices of equations which can be considered for determination of the $\omega$-th subsystem.

Step I. $\{k\} \leftrightarrow \{m \mid m \notin \{s\}\}$

When $\{k\}$ does not include any index out of $\{m\}$, then $\Theta_r + 1 \to \Theta_r$ and the algorithm continues by Step K.

$\Theta_k = \sum_n q_{kn}$

$\{r\} \subset \{k\} : \Theta_r = \min_k [\Theta_k]$

If $\Theta_r > 1$, continue by Step J.

Otherwise let for any $r$ $\Theta_r = q_{ru} = 1$ $(u \in \{n\})$, then $\omega \to \vartheta_r, \eta_u$. Return back to Step H.

Decomposition begins always with equations with the smallest number of explicit variables. Each equation including only one variable (which is not yet coordinated to some subsystem) forms understandably a simulateneously solvable subsystem and can be thus excluded out of following considerations.

Step J. $\{s\} \cap \{r\} \to \{s\}$

$S = \sum_s 1$

If $S < \Theta_r$, return back to Step I.

Otherwise let $\{s\} \leftrightarrow s = s_1, s_2, \ldots, s_S$

By unification of sets $\{s\}$ and $\{r\}$ a set of indices of equations is obtained which are taken into consideration at determination of the $\omega$-th subsystem. The necessary condition for existence of a subsystem is that the number of equations be not smaller than the number of variables with unknown values which appear in these equations. In the oposite case it is obvious that to the considered equations must be coordinated the needed number of other equations even at the cost of eventual increase of the number of variables – see Steps I. and J.

Step K. $0 \rightarrow l$

$S - \Theta_r + 1 \rightarrow l_{max}$

The basic idea of this decomposition method consists in systematic search of complementary equations (their number is $\Theta_r - 1$) to the selected basic equation ($s$-th in sequence from $\{s\}$) so that the total number of equations corresponds to the number of variables with the unknown value (*i.e.* $\Theta_r$). The quantity $s_{l_{max}}$ is the index of the last equation to which it is still possible to find the needed number of complementary equations.

Step L. $l + 1 \rightarrow l$

If $l < l_{max}$, return back to Step I.

$0 \rightarrow R$

$\{\lambda\} \leftrightarrow \lambda = l$

$0 \rightarrow u$

We have not succeeded to select to the $s_1$-th basic equation the needed number of $\Theta_r - 1$ complementary equations and thus it is necessary to pass on to the $s_{1+1}$-th equation as to the basic one. When this equation is in sequence behind equation with the index $s_{l_{max}}$ it is not possible to find the necessary number of equations and it is necessary to include other suitable equations into the selection *i.e.* equations with the next higher number of variables. Otherwise the basic equation is the first possible equation of the searched subsystem with the set of indices $s_{\{\lambda\}}$.

Step M. $u + 1 \rightarrow u$

If $u > R + l_{max} - l + 1$, return back to Step L.

$(l + u) \cap \{\lambda\} \rightarrow \{\xi\}$

$\Phi = \sum_{n} \sum_{\xi} \mathrm{B} q_{s_\xi n}$

If $\Phi < \Theta_r$, return back to Step M.

$\{\xi\} \rightarrow \{\lambda\}, \sum_{\lambda} l - 1 \rightarrow R$. If $R < \Theta_r - 1$, return back to Step M.

$\{p\} \leftrightarrow \{n | \sum_{\lambda} q_{s_\lambda n} \neq 0\}$

$\omega \rightarrow \vartheta_{s_{(\lambda)}}, \eta_{(p)}$. Return back to Step H.

Index $u$ is the index of the next equation following $l$ which can belong into the searched subsystem. Number of equations which in the sequence according to indices from $\{s\}$ follow the $s_{l+u}$-th equation must at least potentially enable to find the missing equations to the total number $\Theta_r$. When the value $u$ is too high from this point of view, the equation with the index $s_l$ is not suitable as the basic equation and it is necessary in this respect to verify another equation (Step L). The quantity $R$ gives the number of equations behind the basic equation which by their number of unknown variables satisfy the value $\Theta_r$ ($s_l$-th equation satisfies this value in any case). Each newly considered equation with index $s_{l+u}$, together with equations with indices $s_{(\lambda)}$ which have already been accepted for the searched subsystem, must be verified as regards the total number of unknowns (quantity $\Phi$). When the determined number of variables does not suit ($\Theta > \Theta_r$), the $s_{l+u}$-th equation is interchanged with the next equation (Step M). Otherwise this equation is accepted and according to the value of $R$ another needed equation is added to the already accepted equations or the searched subsystem is already found. In the last case all equations of subsystem and variables whose value can be found by solution of the subsystem are properly denoted by the decomposition level $\omega$.

Total number of found subsystems is $\Omega$, individual subsystems are solved in the sequence of values $\omega$ and the $\omega$-th subsystem can be formally denoted as

$$f_{\{m_\omega\}}(x_{\{n_\omega\}}) = 0$$

$$\{m_\omega\} \leftrightarrow \{i | \vartheta_i = \omega\}$$

$$\{n_\omega\} \leftrightarrow \{j | \eta_j = \omega\}$$

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

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

$$\omega = 1, \ldots, \Omega .$$

Example of Application of the Proposed Algorithm

The functioning of the described algorithm in analysis of a chemical engineering system, modelled by a system of algebraic equations, can be illustrated by the system mixer–heat exchanger–mixer[2]. Model of this system is formed by a system of 21 algebraic equations with 36 variables; 9 equations are linear, other equations are nonlinear. Here we are neither interested in the concrete form of equations nor in the process which they describe, and suffices only the occurrence matrix given in Table I. Thus: $N = 36$, $L = 21$, $M = 9$, linear equations have (in the sense of algorithm construction) indices within the range 1 to $M$. System is formed by both types or equations ($\pi = 3$) and includes $N - L = 15$ free variables so that the problem can be solved eventually also as the controlled (optimal) simulation ($\tau = 1$). Values of variables $x_{30}$ to $x_{36}$ must be always known in advance before the solution of the system of equations is started. These variables will be thus apriori considered as control variables, *i.e.* $\gamma_i = 1$ for $i = 30, \ldots, 36$.

By application of the first part of algorithm (Steps A – F) the output variables of equations (for linear equations are they given in Table II) and control variables which are $x_{10}$, $x_{11}$, $x_{17}$, $x_{18}$, $x_{24}$, $x_{26}$, $x_{27}$, $x_{29}$ to $x_{36}$ (*i.e.* $\gamma_j = 1$ for $j = 10, 11, 17, 18, 24, 26, 27, 29, \ldots, 36$) were determined. By solving the linear subsystem dependences are obtained

$i = 1$: $x_8(x_7) = 0$

2: $x_{13}(x_{12}) = 0$, resp. $x_{13}(x_{12}(x_7)) = 0$ or $x_{13}(x_7) = 0$

3: $x_{16} = \text{const.}$

4: $x_{22}(x_{19}, x_{20}, x_{21}) = 0$

5: $x_2(x_4, x_6) = 0$, resp. $x_2(x_4(x_{10}), x_6(x_{11})) = 0$ or $x_2(x_{10}, x_{11}) = 0$

6: $x_{12}(x_7) = 0$

7: $x_6(x_{11}) = 0$

8: $x_4(x_{10}) = 0$

9: $x_{15}(x_{11}, x_{18}) = 0$

from which there results that only

$$a'_{1,7},\ a'_{2,7},\ a'_{4,19},\ a'_{4,20},\ a'_{4,21},\ a'_{5,10},\ a'_{5,11},\ a'_{6,7},\ a'_{7,11},\ a'_{8,10},\ a'_{9,11},\ a'_{9,18}$$

are in general differing from zero. Reduced occurrence matrix is given in Table III (columns of control variables are for simplicity left out — control variables cannot affect the following decomposition, in the very calculation the binary variables $\gamma_j$ serve for their indication.

Solution of the system of equations for the system mixer–heat exchanger–mixer according to the reached system decomposition and selection of variables is demonstrated in the next scheme: $x_j$ variables with the yet unknown value, $\bar{x}_j$ variables with the calculated value, $\bar{\bar{x}}_j$ control variables with the given value:

$$x_2(\bar{\bar{x}}_{10}, \bar{\bar{x}}_{11}) = 0 \rightarrow \bar{x}_2$$

$$x_4(\bar{\bar{x}}_{10}) = 0 \rightarrow \bar{x}_4$$

$$x_6(\bar{\bar{x}}_{11}) = 0 \rightarrow \bar{x}_6$$

TABLE I

Occurrence matrix of the system mixer–heat exchanger–mixer ($f_i$, $x_j$)

| $i$ | $j$ | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 |
| 1 | | | | | | | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 2 | | | | | | | | | | | | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | |
| 3 | | | | | | | | | | | | | | | | 1 | | | | | | | | | | | | | | | | | | | | |
| 4 | | | | | | | | | | | | | | | | | | | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | |
| 5 | | 1 | | 1 | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 6 | | | | | | | 1 | | | | | 1 | | | | | | | | | | | | | | | | | | | | | | | | |
| 7 | | | | | | 1 | | | | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | |
| 8 | | | | 1 | | | | | | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 9 | | | | | | | | | | | 1 | | | | 1 | | | 1 | | | | | | | | | | | | | | | | | | |
| 10 | | 1 | | 1 | | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | 1 | 1 | | | | | |
| 11 | 1 | 1 | 1 | 1 | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 12 | | | | | | 1 | | | | | | | | | | | | | | | | | 1 | 1 | | | | | | | | | | | | |
| 13 | | | | | 1 | 1 | | | | | 1 | | | | | | | | | | | | | | | | | | | | | 1 | | | | |
| 14 | | | 1 | 1 | | | | | 1 | 1 | | | | | | | | | | | | | | | | | | | | | | | | | | |
| 15 | | | 1 | | 1 | | | | 1 | | | | | | | | | | | | | | | | | | | | | | | 1 | | | | |
| 16 | | | | | | | | | | | | | | | | | | | | | | | | | 1 | 1 | 1 | | | | | | | | | |
| 17 | | | | | | | | | | | 1 | 1 | | | 1 | | | 1 | 1 | | | | | | | | | | | | | | 1 | | | |
| 18 | | | | | | | | | | | 1 | | 1 | | 1 | | | 1 | | 1 | | | | | | | | | | | | | | 1 | | |
| 19 | | | | | | | | | | | 1 | | | | 1 | | | 1 | | | 1 | | | | | | | | | | | | | | 1 | 1 |
| 20 | | | | | | | | | | | 1 | | | 1 | 1 | | 1 | 1 | | | | | | | | | | | | | | 1 | | | | |
| 21 | | | | | | | | | | | 1 | | | | | | | | | | | | | | | | | 1 | 1 | | | | | | | |

$$x_{15}(\bar{x}_{11}, \bar{x}_{18}) = 0 \rightarrow \bar{x}_{15}$$

$$x_{16} = \text{const.} \rightarrow \bar{x}_{16}$$

$\omega = 1$: $f_{10}(\bar{x}_2, \bar{x}_4, \bar{x}_6, x_7, \bar{x}_{30}, \bar{x}_{31}) = 0 \rightarrow \bar{x}_7$; $x_8(\bar{x}_7) = 0 \rightarrow \bar{x}_8$; $x_{12}(\bar{x}_7) = 0 \rightarrow \bar{x}_{12}$; $x_{13}(\bar{x}_7) = 0 \rightarrow \bar{x}_{13}$

2: $f_{12}(\bar{x}_6, x_{23}, \bar{x}_{24}) = 0 \rightarrow \bar{x}_{23}$

3: $f_{13}(x_5, \bar{x}_6, \bar{x}_{11}, \bar{x}_{32}) = 0 \rightarrow \bar{x}_5$

4: $f_{16}(x_{25}, \bar{x}_{26}, \bar{x}_{27}) = 0 \rightarrow \bar{x}_{25}$

5: $f_{19}(\bar{x}_{11}, \bar{x}_{15}, \bar{x}_{18}, x_{21}, \bar{x}_{35}, \bar{x}_{36}) = 0 \rightarrow \bar{x}_{21}$

6: $f_{20}(\bar{x}_{11}, x_{14}, \bar{x}_{15}, \bar{x}_{17}, \bar{x}_{18}, \bar{x}_{32}) = 0 \rightarrow \bar{x}_{14}$

TABLE II

Output variables of linear equations

| $i$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|
| $\alpha_i$ | 8 | 13 | 16 | 22 | 2 | 12 | 6 | 4 | 15 |

TABLE III

Reduced occurrence matrix of iterated variables in the subsystem of nonlinear equations $(f_i, x_j)$

| $i$ \ $j$ | 1 | 3 | 5 | 7 | 9 | 14 | 19 | 20 | 21 | 23 | 25 | 28 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 10 | | | | 1 | | | | | | | | |
| 11 | 1 | 1 | 1 | | | | | | | | | |
| 12 | | | | | | | | | | 1 | | |
| 13 | | | 1 | | | | | | | | | |
| 14 | | 1 | | | 1 | | | | | | | |
| 15 | | 1 | 1 | | 1 | | | | | | | |
| 16 | | | | | | | | | | | 1 | |
| 17 | | | | 1 | | | 1 | | | | | |
| 18 | | | | 1 | | | | 1 | | | | |
| 19 | | | | | | | | | 1 | | | |
| 20 | | | | | | 1 | | | | | | |
| 21 | | | | | | | | | | | | 1 |

$$7:\ f_{21}(\bar{x}_{11}, x_{28}, \bar{x}_{29}) = 0 \rightarrow \bar{x}_{28}$$

$$8:\ f_{17}(\bar{x}_{11}, \bar{x}_{12}, \bar{x}_{15}, \bar{x}_{18}, x_{19}, \bar{x}_{33}) = 0 \rightarrow \bar{x}_{19}$$

$$9:\ f_{18}(\bar{x}_{11}, \bar{x}_{13}, \bar{x}_{15}, \bar{x}_{18}, x_{20}, \bar{x}_{34}) = 0 \rightarrow \bar{x}_{20};\ x_{22}(\bar{x}_{19}, \bar{x}_{20}, \bar{x}_{21}) = 0 \rightarrow \bar{x}_{22}$$

$$10:\ \left.\begin{aligned} f_{14}(x_3, \bar{x}_4, x_9, \bar{x}_{10}) &= 0 \\ f_{15}(x_3, \bar{x}_5, x_9, \bar{x}_{32}) &= 0 \end{aligned}\right\} \rightarrow \bar{x}_3, \bar{x}_9$$

$$11:\ f_{11}(x_1, \bar{x}_2, \bar{x}_3, \bar{x}_4, \bar{x}_5, \bar{x}_6) = 0 \rightarrow \bar{x}_1$$

By decomposition of the system of nonlinear equations 11 subsystems were obtained out of which the largest ($\omega = 10$) has the rank equal to 2. High number of control variables (15) is here irrelevant as in the practical case majority of them is not the object of optimisation. It concerns parameters of stable character, such as for inst. rate and composition of the reactants *etc.* Let us note that all information on organization and structure of the simulated system which are necessary for the solution of the system of equations are included only in the occurrence matrix $\boldsymbol{Q}$, vector of output variables of equations $\boldsymbol{\alpha}$, vector of control variables $\boldsymbol{\gamma}$ and vector $\boldsymbol{\vartheta}$ and $\boldsymbol{\eta}$, indicating the relationship of equation and variable to individual subsystems obtained by decomposition of the original system. For determination of values of eliminated variables in dependence on control and iterated variables then serves beside the vector $\boldsymbol{\alpha}$ the vector of constants ($c'_i$) and the matrix of coefficients of linear subsystem ($a'_{ij}$).

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