## GENERATION OF THE SYSTEM OF EQUATIONS FOR EQUATIONALLY ORIENTED GLOBAL SIMULATION OF COMPLEX SYSTEMS

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Generation of the system of equations from equational models of standard unit operations used for solution of global simulation of a complex system in steady state is considered. The procedure is illustrated on a simple example.

In connection with the global, equationally oriented approach to the simulation of complex chemical engineering systems in steady state appears of importance the problem of effective method of construction of the set of equations (in general of algebraic equations) which form the mathematical model of a complex system. The single-purpose construction of the set for each solved problem is suitable for systems whose solution is to be repeated many times without making significant changes in any equation of the model (this case is *e.g.* typical for the research phase of a process, when verification of the complex effect of process parameters and of their changes is concerned *etc.*). For flexible use of computational programms it is necessary to construct the system of equations automatically on basis of equational models of standard unit operations-modules which are at the disposal in the computer library. We generate the set of equations of a system knowing the coincidence of its individual nodes and the form of their model representation by disponibile computational modules.

#### THEORETICAL

The basis for the generation of the system of equations as the mathematical model of a whole complex system is the determination of a unique correspondence among equations/variables of individual modules so that it would be possible-to determine output variables of individual equations and control variables of the system when the optimization problem is concerned; — to solve uniquely in advance the subsystem of linear equations according to their output variables (so — called eliminated variables — first level of system decomposition) and to reduce the original system by substitution for these variables; - to perform the decomposition of the reduced system (in general a subsystem of nonlinear equations) and to determine the hierarchy and sequence of solution of the subsystems determined in this way; - to secure the very solution of individual subsystems of equations in the relation system module

The main carriers of information on system variables and their mutual relations are material streams between the nodes of the system (one of them can represent the vicinity of the system). But the material stream is an aggregated concept, individual elements of its characteristics are: number of phases, number of individual components in a phase, pressure, temperature or a characteristics of economic nature etc. Each of these characteristics can be a variable of the system, but they are coupled with characteristics of chemical physical or mechanical phenomena within the nodeso called internal variables of the module. The basic initial informations on the simulated system are concentrated:

I) in the incidence matrix of nodes  $P = (p_{ij})$ ;  $i, j = 1, ..., N_U$  where  $N_U$  is the number of nodes in the system and where  $p_{ij} = l(\pm 0)$ , if there exists a material stream from the node i to the node j, this stream is denoted by the index l; otherwise there holds  $p_{ii} = 0$ ;

2) in the matrix of coordination node/module  $\mathbf{U} = (u_{ij}) (i = 1, 2; j = 1, ..., N_{ij})$ where  $u_{1,i} = m$  means that to the node j is as a model representant coordinated the module m and where  $u_{2,i} = n$ , means that to the node j is the module m coordinated in the *n*-th rank (by the index of rank *n* is distinguished the multiple coordination of the same module m to several different nodes of the system; differing level of incidence of the node affects in the module the basic parameters of its mathematical model as the number of equations, number of variables etc.);

3) in the matrix of streams  $\mathbf{R} = (r_{1i})(i = 1, ..., N_T; j = 1, ..., N_S; N_T$  is the number of informations concerning the stream and  $N_s$  is the number of streams in the system; out of informations on stream character we are interested first of all in the occurrence of individual phases in the stream, where  $r_{ii} = 1$  if the *i*-th phase appears in the stream j, otherwise  $r_{ii} = 0$ ; i = 1 solid phase, i = 2 liquid phase, i = 3 gaseous phase;  $r_{4i}$  pressure,  $r_{5i}$  temperature (the problem of immiscible liquid for the given node can be considered as some of basic combinations of the heterogeneous mixture -e.g.lighter liquid as gas etc.)

When generating the system of equations of the simulated system we proceed along individual nodes in the direction of natural growth of their index. After calling the corresponding module according to the matrix  $\boldsymbol{U}$  the basic parameters of its model are determined, *i.e.*: number of variables  $N^{m,n}$ , total number of equations  $L^{m,n}$ , number of linear equations  $M^{m,n}$ . As any node of the complex system in its basic process or organisation function represents (or might be formally adapted

so that it would represent) a mixer (several inputs - one output), or splitter (one input - several outputs), or flow system (one input - one output), it is possible to state general rules for hierarchy of variables of material streams and of internal module variables:

1) hierarchy of streams - input streams in the sequence of indices of nodes as their sources, output streams in the sequence of indices of nodes as their receivers; 2) hierarchy of phases - solid phase, liquid phase, gaseous phase; 3) hierarchy of components - sequence of indices of components is fixed and cannot be changed; 4) internal variables of the module with fixed sequence.

Otherwise there holds the rule that the mathematical model of a module must be, with regards to the number of components and incidences among individual nodes of the system, quite general and its dimension can be uniquelly determined on informations of matrices P and R. Unlike the phases the presence of all components in each stream of the system is formally assumed. This has an undisputed advantage in generality, the disadvantage of a certain clumsiness at calculation of the stream branches in which some components do not appear by definition, can be removed by arranging the indices of components into certain separable sequences with individual number of components. The assumption is the representation of such branches by an independent subset of equations which must result also from the following decomposition. Uncomplete sequences of indices of components are not hindering the current indexing of equations and variables of the system. Individual stream branches will consider only components according to separate index sequences which are coordinated to the branches according to the instruction of the special node - separator with a purely organisation function. Separable sequence of indices of components is thus given by the interval on the set of integers  $\langle i_{k1}, i_{k2} \rangle$  where k is the index of sequence,  $i_{k1}$  is the first and  $i_{k2}$  the last index of the sequence and  $i_{k2} - i_{k1} + 1$  is the number of components in the k-th stream branch. The values  $i_{k1}$  and  $i_{k2}$  are given in the form of data in the corresponding module with the respected numerical rank of coordination to the mentioned organisation nodes - separators of branches and in the form of given general principles of hierarchy of material streams.

All bonds among equations and variables of individual nodes/modules and the whole system (by the node/module bond the representation of the node by a module in its certain coordination is understood) are included in the so-called characteristic matrices of equations and variables. Fundamentally the correspondence among indices of modular equations  $F(\mathbf{Y}) = 0$  and system equation  $f(\mathbf{X}) = 0$  and modular variables  $\mathbf{Y}$  and system variables  $\mathbf{X}$  form these matrices. The characteristic matrix of equations  $\alpha(5, L) = (\alpha_{k1}) (k = 1, ..., N_{KE})$ , where  $N_{KE} = 5$  is the number of informations on equation and i = 1, ..., L where L is the total number of equations in the system) includes these informations on equations .1) index of the node in whose

module the equation is located; 2) index of equation in the module at the given coordination; 3) type of equation – linear ( $\alpha \neq 0$ ) of nonlinear ( $\alpha = 0$ ); 4) system index of the output variable of the equation; 5) index of subsystem to which the equation belongs (only in case of nonlinear equation, *i.e.* for  $\alpha = 0$ ).

Information 3) for linear equations gives the numerical order of equation (index of row) in the matrix of coefficients and the vector of constants. The generation of the set of equations itself concern only the informations I), 2) and 3). Informations 4) and 5) are the results of the following decomposition of the system. It is obvious that the relation euqation-node is for each equation unique. With variables is the situation slightly different. When the variables represent a component of internal material stream then it must necessarily appear in modules of two and only of two different nodes – first as the output and second as the input variable. Only variables of external material streams (*i.e.* of the streams from the vicinity into the node of the system and *vice versa*) and internal variables of the module are variables of one model.

The characteristic matric of variables  $\beta(6,N) = (\beta_{kj})$   $(k = 1, ..., N_{KV})$  where  $N_{KV} = 6$  is the number of informations on variable and j = 1, ..., N, where N is the number of variables of the system) includes these informations on variables: 1) index of the first node whose stream is represented by the variable or of that whose model contains the variable as the internal one; 2) modular index of variables see  $\{3, 1\}$ ; 3) index of the second node whose stream is represented by the variable; 4) modular index of variable see  $\{3, 3\}$ ; 5) type of the variable-iterated ( $\beta = 0$ ) or control one ( $\beta = 1$ ); 6) index of subsystem to which the variable belongs (different from zero only with nonlinear iterated variables).

In case the variable belongs to an external material stream or it is internal variable of a module the informations 3) and 4) in the matrix  $\beta$  equal to zero. Information 5) is either given as data of the module or is together with the information 6) obtained at decomposition of the set of equations.

The scheme of generation of set of equations or (which is the same) the construction of characteristic matrices of equations and variables describes the following algorithm.

DATA: 
$$P = (p_{1,k})$$
;  $k = 1, ..., N_U$ ,  $l = 1, ..., N_U$   
 $U = (u_{w,k})$ ;  $w = 1, 2$ ;  $k = 1, ..., N_U$   
 $R = (r_{w,v})$ ;  $w = 1, 2, 3, ..., N_T$ 

 $(N_{\rm T}$  is the number of informations on stream,  $N_{\rm C}$  is the number of components,  $N_{\rm U}$  number of nodes and  $N_{\rm S}$  number of streams in the system; w = 1 solid phase, w = 2 liquid phase, w = 3 gaseous phase)

$$0 \rightarrow k, N'. L', M'$$

Step A.  $k + 1 \rightarrow k$ . If  $k > N_0$ , continue by Step H.  $u_{1,k} \rightarrow m$ ,  $u_{2,k} \rightarrow n$ . CALL MODULE m(k, n). MODULE m(k, n): basing on informations of matrices P, R and quantity  $N_C$ determine, according to the general scheme of the module, the quantities:  $N^{m,n}$  number of variables of the model  $L^{m,n}$  total number of equations of the model and  $M^{m,n}$  number of linear equations of the model. For  $i = 1, ..., L^{m,n}$ ,  $j = 1, ..., M^{m,n}$  and  $l = M^{m,n} + 1, ..., L^{m,n}$ , perform:  $k \rightarrow \alpha_{1,L'+1}$ ;  $i \rightarrow \alpha_{2,L'+1}$ ;  $M' + j \rightarrow \alpha_{3,L'+1}$ ;  $0 \rightarrow \alpha_{3,L'+1}$ ;  $0 \rightarrow t, l, z$ .

Step B.  $l + 1 \rightarrow l$ . If  $l > N_U$ ,  $0 \rightarrow l$ , continue by Step E. If  $p_{1k} = 0$ , return to Step B. If  $l \neq 1$  continue by Step C.  $0 \rightarrow s$ . Continue by Step D.

Step C. 
$$N_C \sum_{w=1}^{3} \left( \sum_{\{1'\}}^{r_{w,p_{1'1}}} + \sum_{\{1'' \le k\}}^{r_{w,p_{11'}}} \right)_{[p_{1'1} \neq 0]}^{|p_{1'1} \neq 0} \to s$$

Step D.  $\sum_{w=1}^{3} r_{w,p_{1k}} \rightarrow v.$ 

For all  $i = 1, ..., vN_c$  and j = t + i perform:  $l \to \gamma_{1,j}$ ;  $s + i \to \gamma_{2,j}$ ;  $0/1 \to \gamma_{3,j}$  (the type of variable is given as data of the module).  $t + vN_c \to t$ . If z = 0, return to Step B.

- Step E.  $l + 1 \rightarrow l$ . If  $l > N_{U}$ , continue by Step F. If  $p_{k1} = 0$ , return into Step E.  $1 \rightarrow z$ ;  $N_{C} \sum_{w=1}^{3} \sum_{\{l' < k\}} r_{w,p_{1},\cdot}|_{p_{1'},1 \neq 0} \rightarrow s$ ;  $\sum_{w=1}^{3} r_{w,p_{k1}} \rightarrow v$ . Return into Step D.
- Step F. If  $t = N^{m,n}$ , continue by step G. For  $j = t + 1, ..., N^{m,n}$  perform:  $0 \to \gamma_{1,j}, 0 \to \gamma_{2,j}, 0/1 \to \gamma_{3,j}$ . Note: the auxiliary matrix  $\gamma$  is common for all modules.

Step G. 
$$\{t\} \leftrightarrow \{j \mid (\beta_{3,J} = k) \cap (\beta_{4,J} = j); J = 1, ..., N'\}; \{i\} \rightarrow \{j \mid j \notin \{t\}\} \Rightarrow$$
  
 $\Rightarrow \{i'\} \leftrightarrow i' = 1, 2, ..., \sum_{(i)} 1; N^{m,n} - \sum_{(i)} 1 \rightarrow \overline{N}^{m,n}; k \rightarrow \beta_{1,N'+i'}; i \rightarrow \beta_{2,N'+i'};$   
 $\gamma_{1,i} \rightarrow \beta_{3,N'+i}; \gamma_{2,i} \rightarrow \beta_{4,N'+i'}; \gamma_{3,i} \rightarrow \beta_{5,N'+i'}$ 

According to the general prescription of the module the modular occurrence matrices (occurrence of modular variables in modular equations), modular matrices

of coefficients and vector of constants of linear equations in auxiliary common matrices  $\gamma$ ,  $\vartheta$  and vector  $\omega$  are constructed. The basis are the informations of system matrices **P** and **R**.

$$\begin{split} \{i\} &\leftrightarrow i = 1, \dots, L^{m,n} ; \quad \{l\} \leftrightarrow l = 1, \dots, M^{m,n} ; \quad \{j\} \leftrightarrow j = 1, \dots, N^{m,n} . \\ I &= L' + i ; \quad K = M' + l \\ 1 &\leq J \leq N' + N^{m,n} \mid (\beta_{i,J} = k) \cap (\beta_{i+1,J} = j) ; \quad t = 1 \text{ or } 3 \end{split}$$

 $\gamma_{ij} \rightarrow q_{II}$  (construction of system occurrence matrix  $\mathbf{Q} = (q_{II})$ );  $\vartheta_{1j} \rightarrow a_{KJ}$ (construction of system matric of coefficients of linear equations  $\mathbf{A} = (a_{KJ})$ );

> $\omega_1 \to c_K$  (construction of system vector constants of linear equations  $C = (c_K)$ );  $N' + \overline{N}^{m,n} \to N'$ ;  $L' + L^{m,n} \to L'$ ;  $M' + M^{m,n} \to M'$ .

Return to Step A.

Step H.  $N' \rightarrow N$  (the number of variables of the system set of equations);

 $L' \rightarrow L$  (the total number of equations of the system set);

 $M' \rightarrow M$  (the number of linear equations of the system set). STOP

The system set of equations is represented by the characteristic matrices of equations  $\alpha$ , variables  $\beta$ , matrix of coefficients of linear equations A and vector of constants of linear equations C. The concrete form of nonlinear equations is given in a a general form in the corresponding modules. The decomposition of the system set is based on the occurrence matrix Q.

The CALL scheme for the equation  $f_1(\mathbf{X}) = 0$  is

$$I \to \alpha_{1,1} : k \to u_{1,k} = m$$

$$\frac{u_{2,k} = n}{f_1(\mathbf{X}) = 0 \leftrightarrow F_{\alpha_{2,1}}^{m,n}(\mathbf{Y}) = 0}$$

The CALL scheme for the variable  $x_J$  is

$$J \rightarrow \beta_{1,J} : k' \rightarrow u_{1,k'} = m'$$

$$u_{2,k'} = n'$$

$$resp. \qquad x_{J} \leftrightarrow y_{\beta_{2,J}}^{m',n'}$$

$$\longrightarrow \beta_{3,J} : k'' \rightarrow u_{1,k''} = m''$$

$$u_{2^{*}k''} = n''$$

$$\overline{x_{J} \leftrightarrow y_{\beta_{4,J}}^{m',n'}}$$

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If the *I*-th equation of the system set is a linear one its coefficients and constant are the elements  $a_{\alpha_{1,1},J}$  and  $c_{\alpha_{3,1}}$  of the matrix **A** and the vector **C**.

#### EXAMPLE

Here is considered generation of the set of equations for simulation of a process which forms a system with seven technological nodes, twelve material streams and three components in three phases. There are 6 modules for the model description of the system: homogeneous mixer (m = 1); heterogeneous mixer (m = 2); chemical reactor (m = 3); homogeneous separator (m = 4); heterogeneous separator m = 5; vicinity of the system (input of raw material and output of product) (m = 6). Modules are coordinated to individual nodes  $(N_U = 7)$  in the order

$$U = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ \hline 6 & 2 & 3 & 5 & 1 & 3 & 4 \\ 2 & 1 & 1 & 1 & 1 & 2 & 1 \end{bmatrix}$$

Incidence matrix of nodes P and the matrix of streams R have the form

General models of considered modules are:

# Homogeneous Mixer (m = 1)

Model of the homogeneous mixer is formed by balance equations of components regardless of phases, so that  $L^{1,n} = M^{1,n} = N_c$ . The number of model variables is given by the relation  $N^{1,n} = N_c(N_s^{1,n} + 1)$ , where

$$\begin{split} N_{\mathsf{S}}^{1,n} &= \sum_{(i')} 1 \; ; \; \{i'\} \leftrightarrow \{i \mid p_{i\mathsf{k}} \neq 0\} \\ \{i\} \leftrightarrow i = 1, ..., N_{\mathsf{U}}, \quad k : u_{1,\mathsf{k}} = m, \quad u_{2,\mathsf{k}} = n \end{split}$$

is the number of input streams into the mixer and  $p_{ik}$  is the element of incidence matric of nodes **P**. With regard to the accepted hierarchy of components and streams

each equation of the model has a general form

$$F_{j}^{1,n}(\mathbf{Y})\sum_{w=1}^{N_{S}^{1,n}} y_{(w-1)N_{C}+j} - y_{N_{C}N_{S}^{1,n}+j} = 0; \quad j = 1, ..., N_{C}$$

The variables with indices 1, ...,  $N_c N_s^{1,n}$  correspond to components of input streams,  $(w - 1) N_c + j$  is the index of *j*-th component in *w*-th input stream and  $N_c N_s^{1,n} + j$ is the index of *j*-th component in the output stream. The occurrence matrix of variables in equations of the module  $\mathbf{Q}^{1,n}(L^{1,n}, N^{1,n})$  has its general element

$$q_{j1}^{1,n} = \begin{cases} 1 & \text{if } l = (w-1)N_{C} + j; & w = 1, ..., N_{S}^{1,n} + 1; \\ 0 & \text{otherwise} \end{cases}$$

Similarly the matrix of coefficients of linear equations is formed by general elements

$$a_{ji}^{1,n} = \begin{cases} 1 & \text{if } l = (u-1) N_C + j ; u = 1, ..., N_S^{1,n} \\ -1 & \text{if } l = N_C N_S^{1,n} + j ; \\ 0 & \text{otherwise} \end{cases}$$

All elements of the vector of constant  $c_i^{1,n}$  are equal to zero.

Homogeneous mixer is a special case of heterogeneous mixer for single-phase flows.

#### Heterogeneous Mixer (m = 2)

i =

Model of the heterogeneous mixer is formed by balance equations of components in individual phases. Here it is assumed that at mixing of streams mass transfer among phases does not take place. The number of equations is  $L^{2,n} = M^{2,n} =$  $= N_C \sum_{w=1}^{3} r_{w,p_{kk'}}$ , where k' is the index of the node into which the output stream from the mixer enters. The total number of module variables is  $N^{2,n} = N_C \sum_{w=1}^{3} (\sum_{i=1}^{N} r_{w,p_{1'k}} +$  $+ r_{w,p_{kk'}}$ ;  $\{i'\} \leftrightarrow \{i \mid p_{ik} \neq 0\}$ ;  $\{i\} \leftrightarrow i = 1, ..., N_U$ ;  $k : u_{1,k} = m, u_{2,k} = n$ 

 $+ r_{\mathbf{w},\mathbf{p}_{\mathbf{k}\mathbf{k}}}; \{i'\} \leftrightarrow \{i \mid p_{i\mathbf{k}} \neq 0\}; \{i\} \leftrightarrow i = 1, ..., N_{\mathbf{U}}; k: u_{1,\mathbf{k}} = m, u_{2,\mathbf{k}} = n$ 

Construction of equations of the model - the balance of *l*-th component in *j*-th phase:

$$\{i'\} \Rightarrow \{j_{i'}\} \leftrightarrow j_{i'} = 1, 2, \dots, N_{S,k}^{2,n} = \sum_{\{i'\}} 1;$$

$$\Phi_0 = 0; \quad \Phi_{j_{1'}} = \Phi_{j_{1'-1}} + N_C \sum_{w=1}^3 r_{w,p_{1'k}};$$

$$1, 2, \dots, \sum_{w=1}^3 r_{w,p_{kk'}}; \quad l = 1, \dots, N_C; \quad r_{0,0} = 0; \quad \alpha(j, l) = (j-1)N_C + l$$

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$$\begin{split} \beta_{j_{1}\cdot}(j,\,l,\,i') &= \left( \Phi_{j_{1}\cdot-1} \,+\, N_{C} \sum_{w=1}^{j} r_{w-1,p_{1}\cdot k} \,+\, l \right) r_{j,p_{1}\cdot k} \left( ! \,\pm\, 0 \right) \,; \\ \gamma(j,\,l) &=\, \Phi_{N_{s,k}2,n} \,+\, (j\,-\,1) \,N_{C} \,+\, l \,=\, \Phi_{N_{s,k}2,n} \,+\, \alpha(j,\,l) \\ F_{\alpha(j,1)}^{2,n}(\mathbf{Y}) &=\, \sum_{j_{1}\cdot\, z=\, 1}^{N_{s,k}2,n} \,y_{\beta_{j_{1}\cdot}(j,1,i')} \,-\, y_{\gamma(j,1)} \,=\, 0 \;. \end{split}$$

The variable with the index  $\beta_{j_1}$ , (j, l, i') corresponds to the *l*-th component in the *j*-th phase of the input stream (i', k), which is the  $j_i'$ -th input stream in the numerical order. The variable with the index  $\gamma(j, l)$  corresponds to the *l*-th component in the *j*-th phase of the output stream. When constructing the equations of the heterogeneous mixer model we have to keep in mind that the phase is made superior over the component, *i.e.* that the index *l* takes all its values for the given *j* continuously. Occurrence matrix of variables in equations  $\mathbf{Q}^{2,n}(L^{2,n}, 3, N^{2,n})$  has the generally defined element

$$q_{s(j,1),v}^{2,n} = \begin{cases} 1 & \text{if } v = \beta_{j_1, \cdot} (j, l, i') (! \neq 0) & \text{or } v = \gamma (j, l); \\ 0 & \text{otherwise}. \end{cases}$$

An element of the matrix A<sup>2,n</sup> is defined as

$$a_{a(j,1),v}^{2,n} = \begin{cases} 1 & \text{if } v = \beta_{j_1}, (j, l, i') (! \neq 0); \\ -1 & \text{if } v = \gamma(j, l); \\ 0 & \text{otherwise}. \end{cases}$$

 $v = 1, ..., N^{2,n}$ 

All elements of vector  $C^{2,n}$ , *i.e.*  $c_{\alpha(j,1)}^{2,n}$ , have their values equal to zero.

Reactor (m = 3)

Model of the reactor of our illustrative example is considered only in a special form of a set of nonlinear algebraic equations

$$\begin{split} F_{i}^{3,n}(\mathbf{Y}) &= 0 \; ; \quad i = 1, \dots, N_{C} \sum_{j=1}^{3} r_{j,p_{kk}} ; \\ L^{3,n} &= N_{C} \sum_{j=1}^{3} r_{j,p_{kk'}} ; \\ M^{3,n} &= 0 \; ; \\ N^{3,n} &= N_{C} \sum_{j=1}^{3} (r_{j,p_{k''k}} + r_{j,p_{kk'}}) \; , \end{split}$$

where the stream (k'', k) is the input one and (k, k') is the output stream of the reactor.

The variables with indices  $j = 1, ..., N_C \sum_{j=1}^{3} r_{j, p_k \cdots_k}$  correspond to the components of the input stream of the reactor and the variables with indices

$$j = N_{C} \sum_{j=1}^{3} r_{j, p_{k''k}} + 1, ..., N_{C} \sum_{j=1}^{3} (r_{j, p_{k''k}} + r_{j, p_{kk}})$$

correspond to the components of its output stream. The occurrence matrix is fully occupied by nonzero elements.

Homogeneous Separator (m = 4)

Here

$$\begin{split} N_{\rm S}^{4,n} &= \sum_{(i')} 1 \quad \{i'\} \leftrightarrow \{i \mid p_{kl} \neq 0\} ; \\ \{i\} \leftrightarrow i = 1, \dots, N_{\rm U} ; \quad k : u_{1,k} = m , \quad u_{2,k} = n \end{split}$$

is the number of output streams from the separator.

$$L^{4,n} = N_{\rm C} N_{\rm S}^{4,n} + 1$$
;  $M^{4,n} = 1$ ;  $N^{4,n} = (N_{\rm S}^{4,n} + 1) N_{\rm C} + N_{\rm S}^{4,n}$ 

If  $N_c j$  + i is the index of *i*-th component in *j*-th output stream  $N_c(N_s^{4,n} + 1) + j$  is the index of separation ratio of the *j*-th output stream and *i* is the index of *i*-th component in the input stream, then the model of the separator is formed by equations

$$F_1^{4,n}(\mathbf{Y}) = \sum_{j=1}^{N_S^{4,n}} y_{N_C(N_S^{4,n+1})+j} - 1 = 0$$

and

l

$$\begin{split} F^{4,n}_{(j-1)N_C+i+1}(\mathbf{Y}) &= y_{N_C(N_S^{4,n+1})+j} \cdot y_i - y_{N_Cj+i} = 0\\ i &= 1, \dots, N_C; \quad j = 1, \dots, N_S^{4,n} \,. \end{split}$$

For the elements of the occurrence matrix there holds

$$q_{1,v}^{4,n} = \begin{cases} 1 & \text{if } v = N_{\rm C}(N_{\rm S}^{4,n} + 1) + j; \\ 0 & \text{otherwise}; \end{cases}$$

$$l_{(j-1)N_{\rm C}+i+1,v}^{4,n} = \begin{cases} 1 & \text{if } v = N_{\rm C}(N_{\rm S}^{4,n} + 1) + j & \text{or } v = i. \text{ or } v = N_{\rm C}j + i; \\ 0 & \text{otherwise}. \end{cases}$$

Similarly

$$a_{1,v}^{4,n} = \begin{cases} 1 & \text{if } v = N_{\rm C}(N_{\rm S}^{4,n} + 1) + j; \\ 0 & \text{otherwise}; \end{cases}$$
$$c_{1,n}^{4,n} = -1.$$

#### Heterogeneous Separator (m = 5)

The function of heterogeneous separator rests in the separation of some or of all phases of the input stream.

$$\Phi = \sum_{\mathbf{w}=1}^{3} r_{\mathbf{w},\mathbf{p}_{\mathbf{k}',\mathbf{k}}}$$

is the number of phases in the input stream (k', k) into the separator;  $L^{5,n} = M^{5,n} = = \phi N_C$ ;  $N^{5,n} = 2\phi N_C$ . Index of variable – component of input stream is (j - 1). .  $N_C + i$ . Index of variable – component of output stream is  $(\phi + j - 1)N_C + i$  $j = 1, ..., \phi$ ;  $i = 1, ..., N_C$ 

$$F_{(j-1)N_{c}+i}^{5,n}(Y) = y_{(j-1)N_{c}+i} - y_{(\Phi+j-1)N_{c}+i} = 0.$$

The occurrence matrix  $\mathbf{Q}^{5,n}(L^{5,n}, N^{5,n})$  is defined as

 $q_{wv}^{5,n} = \begin{cases} 1 & \text{if } v = w & \text{or } v = \Phi N_{C} + w \\ 0 & \text{otherwise} . \end{cases}$ 

The matrix of coefficients of linear equations  $A^{5,n}$ :

$$a_{\mathbf{w},\mathbf{v}}^{5,n} = \begin{cases} 1 & \text{if } v = w ; \\ -1 & \text{if } v = \Phi N_{C} + w ; \\ 0 & \text{otherwise} . \end{cases}$$

The elements of the vector of constants  $c_j^{5,n}$  are equal to zero.

# The Vicinity of the System (m = 6)

Here are indexed only the components of input and output streams, *i.e.* input from the vicinity and output to the vicinity of the complex system.

There holds  $L^{7,n} = M^{7,n} = 0$  and  $N^{7,n} = \Phi N_{\rm C}$ , where

$$\Phi = \sum_{\mathbf{w}=1}^{3} \left( \sum_{\{i'\}} e_{\mathbf{w}, p_{1'\mathbf{k}}} + \sum_{\{i''\}} r_{\mathbf{w}, p_{\mathbf{k}1''}} \right) \quad \{i'\} \leftrightarrow \{i \mid p_{i\mathbf{k}} \neq 0\} ,$$

$$\{i''\} \leftrightarrow \{i \mid p_{k1} \neq 0\}; \{i\} \leftrightarrow i = 1, ..., N_{U}; u_{1,k} = m, u_{2,k} = n\}.$$

The Generation of the System Set of Equations

1

$$L' = M' = N' = 0; \quad k = 0.$$

$$\rightarrow k : Node 1$$

$$u_{1,1} = 6 \rightarrow m$$

$$u_{2,1} = 1 \rightarrow n$$

$$\overline{L^{6,n} = 0 \text{ (the matrix } \alpha \text{ is not considered)} }$$

 $2 \rightarrow k$ : Node 2

~

$$u_{1,2} = 2 \rightarrow m$$

$$u_{2,2} = 1 \rightarrow n$$

$$L^{2,1} = M^{2,1} = N_C \sum_{w=1}^{3} r_{w,p_{2,3}} = N_C \sum_{w=1}^{3} r_{w,3} = 3(1+1+0) = 6$$

Equationally Oriented Global Simulation of Complex Systems

$$N^{2,1} = N_C \sum_{w=1}^{3} \left[ \left( r_{w,1} + r_{w,5} + r_{w,10} \right) + \left( r_{w,3} \right) \right] = 18$$

 $i = 1, ..., 6; j = 1, ..., 6; \{l\} = empty set of indices (L<sup>2,1</sup> = M<sup>2,1</sup>)$ 

									ł	2 3	8 4	5 6	i						
						d	t ==	= 1 2 3	2 1 1	2 2 2	2 2 3 4 3 4	2 5 5	2 6 6						
		I	2	3	4	5	6	7	8	9	10	П	12	13	14	15	16	17	18
γ =	1	1	1	1	1	I	1	4	4	4	7	7	7	3	3	3	3	3	3
	2	1	2	3	4	5	6	13	14	15	7	8	9	1	2	3	4	5	6
	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
				k	, ,	<	2 -	→ Ī	<b>⊽</b> ².	' =	- 18	3 -	6	=	12				

k = 2: the second row and second column of matrix **P** are checked. According to the number of stream (k', k) or (k, k') number of phases in the stream is found in the matrix **R**. For k' < 2 (*i.e.* 1) from the already formed matrix  $\beta$  (by comparison of the first and third row) the modular indices of the variables of the node 1 are determined. Similarly for nodes 4 and 7. *E.g.* the variables of the stream (4, 2) must by indices correspond to the variables of the stream (4,1).

Matrix  $\mathbf{Q}^{2,o}$  is constructed in agreement with the prescription according to the increasing *l* within the increasing *j*:  $i' = 1, 4, 7; j_{i'} = 1, 2, 3$ .

$$\Phi_{0} = 0$$

$$\Phi_{1} = \Phi_{0} + N_{C} \sum_{w=1}^{3} r_{w,p_{1,2}} = 6$$

$$\Phi_{2} = \Phi_{1} + N_{C} \sum_{w=1}^{3} r_{w,p_{1,2}} = 9 \quad ((2, k') = (2, 3), \quad \sum_{w=1}^{3} r_{w,p_{2,3}} = 2) \Rightarrow j = 1, 2$$

$$\Phi_{3} = \Phi_{2} + N_{C} \sum_{w=1}^{3} r_{w,p_{1,2}} = 12 \quad ((N_{S,2}^{2.1}) = 3)$$

$$= 7, 8, 9, 10, 11, 12, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27$$

•••		10 1		2 10	, , ,	10 .				2.5 2			.0 .	
Q = 1	1				1				1					
2	1				1					1				
3	1					1					ł			
4		1					1					1		
5			1					1					1	
6				1					1					I
÷														

Similarly

... 7 8 9 10 11 12 16 17 18 19 20 21 22 23 24 25 26 27 ...  $\mathbf{A} = \mathbf{1}$ 1 1 -- 1 2 --- 1 1 1 - 1 3 1 1 -14 1 1 5 -11 1 6 --- 1 1 1  $\mathbf{C}^{T} = 1 \ 2 \ 3 \ 4 \ 5 \ 6$ 0 0 0 0 0 0  $N' + \overline{N}^{2,1} = 15 + 12 = 27 \rightarrow N'$  $L' + L^{2,1} = 0 + 6 = 6 \rightarrow L'$  $M' + M^{2,1} = 0 + 6 = 6 \rightarrow M'$ 

 $3 \rightarrow k$ : Node 3

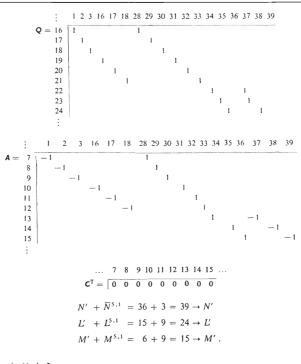
$u_{1,3} = 3 \rightarrow m$
$u_{2,3} = 1 \rightarrow n$
$L^{3,1} = N_C \sum_{j=1}^{3} r_{j,p_{3,4}} = 9$
$M^{3.1} = 0$
$N^{3.1} = N_C \sum_{j=1}^{3} (r_{j,p_{2,3}} + r_{j,p_{3,4}}) = 15$
7 8 9 10 11 12 13 14 15
$\alpha = 1$ 3 3 3 3 3 3 3 3 3 3 3
$ \alpha = 1 \begin{bmatrix} 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3 & 3$
3 0 0 0 0 0 0 0 0 0
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
$y = 1 \begin{vmatrix} 2 & 2 & 2 & 2 & 2 & 2 & 2 & 4 & 4 & 4 &$
$y = 1 \begin{vmatrix} 2 & 2 & 2 & 2 & 2 & 2 & 2 & 4 & 4 & 4 &$
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$y = 1 \begin{vmatrix} 2 & 2 & 2 & 2 & 2 & 2 & 4 & 4 & 4 & 4 &$
$y = 1 \begin{bmatrix} 2 & 2 & 2 & 2 & 2 & 2 & 4 & 4 & 4 & 4 &$
$y = 1 \begin{vmatrix} 2 & 2 & 2 & 2 & 2 & 2 & 4 & 4 & 4 & 4 &$

From the full occupation of matrix  $Q^{3,1}$  by nonzero elements results

	:	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	
<b>Q</b> =	7	1	1	1	i	1	ł	1	1	1	1	1	1	1	I	1	
	8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
	9	1	1	1	1	1	1	1	ł	1	1	1	1	1	1	1	
	10	1	1	1	1	1	Ι	1	1	1	1	1	1	J	Т	1	
	П	1	1	1	1	1	1	1	1	1	i	ł	1	1	1	1	
	12	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
	13	1	1	1	1	1	1	1	1	1	1	ł	1	1	1	1	
	14	j.	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
	15	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	
	:																

$$\begin{split} N' &+ \overline{N}^{3.1} &= 27 + 9 = 36 \to N' \\ L' &+ L^{3.1} &= 6 + 9 = 15 \to L'^1 \\ M' &+ M^{3.1} &= 6 + 0 = 6 \to M' \,. \end{split}$$

 $4 \rightarrow k$ : Node 4



 $5 \rightarrow k$ : Node 5

$$\begin{array}{l} u_{1,5} = 1 \rightarrow m \\ u_{2,5} = 1 \rightarrow n \\ \hline U^{1,1} = M^{1,1} = 3 \\ i' = 1, 4, 7 \rightarrow N_{\rm S}^{1,1} = 3 \\ N^{1,1} = 3(3+1) = 12 \,. \end{array}$$

 $6 \rightarrow k$ : Node 6

$$u_{1,6} = 3 \to m$$
  

$$u_{2,6} = 2 \to n$$
  

$$L^{3,2} = 3 \cdot 1 = 3$$
  

$$M^{3,2} = 0$$
  

$$N^{3,2} = 3(1 + 1) = 6$$

$\alpha = 1 \begin{bmatrix} 6 & 6 & 6 \\ 1 & 2 & 3 \\ 2 & 1 & 2 & 3 \\ 3 & 0 & 0 & 0 \end{bmatrix}$
$y = 1 \qquad \begin{array}{ccccccccccccccccccccccccccccccccccc$
$\mathbf{Q} = \begin{array}{ccccccccccccccccccccccccccccccccccc$
$\begin{array}{rcl} N' &+ \overline{N}^{3,2} &= 45 + 3 = 48 \rightarrow N' \\ L' &+ L^{3,2} &= 27 + 3 = 30 \rightarrow L' \\ M' + M^{3,2} = 18 + 0 = 18 \rightarrow M' \end{array}$

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 $7 \rightarrow k$ : No

By application of the first phase of the decomposition algorithm<sup>1</sup> on the occurrence matrix  $\mathbf{Q}$  the output variables of linear equations are determined.

and of control variable:  $x_{22}$ ,  $x_{23}$ ,  $x_{24}$ ,  $x_{25}$ ,  $x_{26}$ ,  $x_{27}$ ,  $x_{34}$ ,  $x_{35}$ ,  $x_{36}$ ,  $x_{50}$ ,  $x_{51}$ .

Let us remind that to the linear equations with the system index *i* in the matrix **Q** corresponds the index of the subsystem of linear equations  $\alpha_{3,i}$  in the matrix of coefficients **A**; by a single solution of the linear subsystem the dependences (LSS) are obtained:

$$\begin{aligned} x_1 &= x_{28} \\ x_2 &= x_{29} \\ x_3 &= x_{30} \\ x_7 &= -x_{16} + x_{22} = x_{22} - x_{31} \\ x_8 &= -x_{17} + x_{23} = x_{23} - x_{32} \\ x_9 &= -x_{18} + x_{24} = x_{24} - x_{33} \\ x_{10} &= -x_{19} + x_{25} \\ x_{11} &= -x_{20} + x_{26} \\ x_{12} &= -x_{21} + x_{27} \\ x_{13} &= -x_{34} - x_{40} + x_{43} \\ x_{14} &= -x_{35} - x_{41} + x_{44} \\ x_{15} &= -x_{36} - x_{42} + x_{45} \\ x_{16} &= x_{31} \\ x_{17} &= x_{32} \\ x_{18} &= x_{33} \\ x_{37} &= x_{34} \\ x_{38} &= x_{35} \\ x_{39} &= x_{36} \\ x_{49} &= 1 - x_{50} - x_{51} \end{aligned}$$

By application of the second phase of decomposition algorithm<sup>1</sup> the following scheme of solution of the system of equations is obtained:

LSS j 37 (34,) 38 (35,) 39 (36), 49 (50, 51) – depends only on control equation i 7, 8, 9, 10, 11, 12, 13, 14, 15 –  $\alpha_{5,i} = 1$ variables j 16 (31), 17 (32), 18 (33), 19, 20, 21, 28, 29, 30, 31, 32, 33, 34 (control), 35 (control), 36 (control) –  $\beta_{6,j} = 1$ LSS j 1 (28), 2 (29), 3 (30), 7 (22, 31), 8 (23, 32), 9 (24, 33), 10 (19, 25), 11 (20, 26), 12 (21, 27), 16 (31), 17 (32), 18 (33) equation i 35 –  $\alpha_{5,i} = 2$ variables j 19 (known), 46, 50 (control) –  $\beta_{6,j} = 2$ equation i 36 –  $\alpha_{5,i} = 3$ variables j 20 (known), 47, 50 (control) –  $\beta_{6,j} = 3$ 

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equation i  $37 - \alpha_{5,i} = 4$ variables j 21 (known), 48, 50 (control) -  $\beta_{6i} = 4$ equation i  $32 - \alpha_{5,i} = 5$ variables j 4, 46 (known), 39 (50 - control, 51 - control) -  $\beta_{6,1} = 5$ equation i 33 -  $\alpha_{5,i} = 6$ variables j 5, 47 (known), 49 (50 - control), 51 - control) -  $\beta_{6,i} = 6$ equation i  $34 - \alpha_{5,i} = 7$ variables j 6, 48 (known), 49 (50 - control, 51 - control) -  $\beta_{6,1} = 7$ equation i  $38 - \alpha_{5,i} = 8$ variables j 40, 46 (known), 51 (control) -  $\beta_{6,i} = 8$ equation i 39 -  $\alpha_{5i} = 9$ variables j 41, 47 (known), 51 (control) –  $\beta_{6,1} = 9$ equation i  $40 - \alpha_{5,i} = 10$ variables j 42, 48 (known), 51 (control) –  $\beta_{6,j} = 10$ equation i 28, 29, 30 -  $\alpha_{5,i} = 11$ variables j 43, 44, 45, 46 (known), 47 (known), 48 (known) -  $\beta_{6,i} = 11$ LSS j 13 (34, 40, 43), 14 (35, 41, 44), 15 (36, 42, 45)

#### REFERENCES

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Translated by M. Rylek.