CHEMICAL PROCESSES SIMULATION PROGRAMS — PRESENT STATE AND FUTURE DEVELOPMENT OF FLOWSHEETING

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Basic information on 14 programming systems for simulation of chemical processes in steady state are reviewed. An important part are simulation programs originated in CMEA countries which have not yet been covered in a comprehensive study. On basis of an analysis an attempt has been made to ascertain the present and future trends of development. There are some supplementary information on two balancing programs and two systems for dynamic simulation of chemical processes which solve problems from a slightly different category. However, they are also important modules necessary for construction of programming systems for computer aided design.

Simulation of chemical processes, which is here understood as a mathematical modelling of a process (in our case in the steady state) represented by the flowsheet, is solved on the digital computer by use of specialized programs or more general simulation programming systems. (Some authors *e.g.* Rudd and Watson[1] are using terms "simulation languages" or "macrolanguages" Briddell[2]). The term "general" should be understood with certain limitation; these systems solve certain class of problems – as wide as possible. One-purpose programs have some advantages, *e.g.* they are closely tailored to a specific process, but also some disadvantages too. Namely they are suitable only for one individual invariable process; this usually causes their higher costs due to a rather long time-consuming preparation. This is why the general-purpose programming systems are usually preferred by organizations concerned with several different processes (Kehat and Shacham[3]).

The basic question which must be solved while developing the general-purpose program is the selection of the concept *i.e.* of the equation-oriented or modular approach.

The equation-oriented approach used *e.g.* by Sargent and Westerberg[4] is at present less frequent. In its application we consider the solution of a system of nonlinear equations describing the behaviour of the process without distributing them into modules corresponding to individual models of process units. The advantage is the possibility to solve relatively easily also the balancing-simulation problems. The considerable disadvantage is the lesser clarity of presentation and more complex mani-

pulation when the need for changes of the process units or in the topology of the process is raised provided the problems with own solution of complex systems of nonlinear equations are not considered.

The majority of simulation systems is using the modular approach (Johnson[5]). The basic principle is that to the unit operation or to the unit process taking place in the apparatus corresponds the "unit calculation" – the module (Crowe and co-workers[6]). The model of the whole process is then composed from unit calculations. This arrangement corresponds both to the deep-rooted procedures in the process design calculations and to the modular structure of the used higher programming languages (ALGOL, FORTRAN, PL/1).

In connection with the structure of programming languages the simulation systems are built modulary also on other levels *e.g.* the simulation programming system is a module itself in an integrated computer aided design system[7]. There is also a possibility to compose the unit calculations from the modules of lower levels. In general the greatest advantage of the modular approach is the great flexibility and expediency, *i.e.* the characteristics which far counter balance some difficulties encountered when complex algorithms are developed.

Specification of Basic Terms

Most of the basic terminology is generally known and is used in the same sense by the majority of authors. Thus such terms as mathematical model, simulation, simulation system, chemical process, process and information flowsheet, nodes, streams, parameters of process units, balanced components *etc.* are not specified here in detail; their definitions can be found in literature[6,8–10]. However, to avoid misunderstanding, it has been thought appropriate to classify the problem of mathematical modelling on basis of their formulation and specification, *i.e.* according to the selection of the independent variables and of the mathematical apparatus used.

Let $\mathscr{K}$ is the set of information flowsheet (the graph) nodes having K elements and $\mathscr{P}$ the set of its branches (streams) having P elements. The streams are representing the flow rate of balanced quantities and/or other information; it is assumed that no changes occur in streams. To the stream leaving the node i and entering the node j is assigned the specification vector $\boldsymbol{S}_{ij}$. The components of this vector are flow rates of all balanced components (mass and heat flow rates) and some other information *e.g.* the pressure values. The specification vector is given by

$$\boldsymbol{S}_{ij} = (S_{ij}^1, S_{ij}^2, \ldots, S_{ij}^F, S_{ij}^{F+1}, \ldots, S_{ij}^{F+1+G}) \qquad (i)$$

where F is the number of balanced mass components, F + 1st component of vector

represents the heat flow, G is the number of other information (*e.g.* the pressure).

The set of specification vectors of all streams entering the i-th node is

$$\{\boldsymbol{S}_{xi}\} = \mathscr{X}_i \quad xi \in \mathscr{N}_i \tag{2}$$

where $\mathscr{N}_i$ is the set of all streams entering the node i and the number of its elements N is related to the aforementioned sets as follows: $N \leqq K \leqq P$.

Similarly for streams leaving the i-th node the set of specification vectors is defined as

$$\{\boldsymbol{S}_{iy}\} = \mathscr{Y}_i \quad iy \in \mathscr{M}_i \tag{3}$$

where $\mathscr{M}_i$ is the set of streams leaving the node i and the number of its elements is $M \leqq K \leqq P$. Obviously it also holds

$$\mathscr{N}_i \subset \mathscr{P} \quad i \in \mathscr{K} \tag{4}$$

or

$$\mathscr{M}_i \subset \mathscr{P} \quad i \in \mathscr{K} \tag{5}$$

Each node of the flowsheet represents a certain transformation (for which *e.g.* Kafarov, Perov and Meshalkin[9] introduce the term "multidimensional technological operator") which assigns to the set $\mathscr{X}_i$ the set of vectors $\mathscr{Y}_i$

$$\mathscr{Y}_i = \Phi(\mathscr{X}_i, \boldsymbol{D}_i), \tag{6}$$

where $\boldsymbol{D}_i$ is the vector of variables (parameters of the process units) having the control of the transformations which belong to the node i – see Fig. 1.

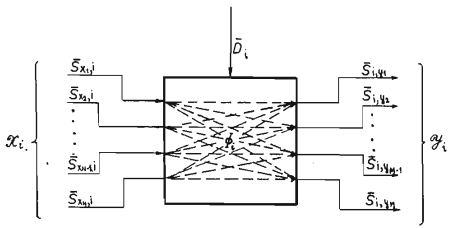

FIG. 1

Transformation Represented by the Flowsheet Node

The set of transformations $\mathscr{F} = \{\Phi_i\}$; $i \in \mathscr{K}$ is essentially the set of mathematical models of the process unit. The environment of the process is assumed as zero node. Then the number of nodes is usually equal to the number of physical apparatuses plus one, but in general one node can correspond to several apparatuses and vice versa, according to the construction of the actual model. The vectors $\boldsymbol{S}_{0i}$ and $\boldsymbol{S}_{i0}$ are describing the streams entering and leaving the modelled process (feed and products).The graph of the process is then cyclical if each node (including the zero node) is the location of incidence of two or more streams; so $\boldsymbol{S}$ it holds that

$$\forall i, j \in \mathscr{K} \;\; \exists xj \in \mathscr{N}_j \;\; \exists iy \in \mathscr{M}_i \left[\boldsymbol{S}_{xy} \in \mathscr{X}_j \wedge \boldsymbol{S}_{xy} \in \mathscr{Y}_i\right]. \tag{7}$$

For individual elements of the sets $\mathscr{X}_j$ and $\mathscr{Y}_i$ corresponding to the nodes i and j connected by the stream ij holds

$$\left[\mathscr{X}_j\right]_i \equiv \left[\mathscr{Y}_i\right]_j \equiv \boldsymbol{S}_{ij} \quad i, j \in \mathscr{K}. \tag{8}$$

Relations (7) and (8) incorporate also the case of the stream returning to the same node ($i \equiv j$).

This graph can be described by the set $\mathscr{T}$ depicting the mutual relations of nodes, *e.g.* by the process matrix or by the stream connection matrix.

Simulation problem is then defined: Let the following input data are specified

a) Data on the process topology – the set of relations $\mathscr{T}$,

b) set $\mathscr{Y}_0$ of specification vectors of streams entering the modelled process,

c) transformations of all nodes – the set $\mathscr{F}$, *i.e.* mathematical models of the process units,

d) set $\mathscr{D} = \{\boldsymbol{D}_i\}$, $i \in \mathscr{K}$ of process units parameters (in simulation they are the independent variables)

– the calculation returns the overall mass and heat balance on the chemical process *i.e.* flow rates of all balanced quantities – the sets of specification vectors of streams $\mathscr{Y}_i$, $i \in \mathscr{K}$.

(The problem so defined has a unique solution).

The balancing problem is qualitatively different from the simulation one; although the results give again the flow rates of all balanced quantities (the sets $\mathscr{Y}_i$, $i \in \mathscr{K}$ are determined) the models of nodes do not enter the picture. Formally and practically it is possible to express this problem so that the transformations $\mathscr{F}$ are reduced to linear relations describing the fact that in the node – in the point of incidence of streams – the sum of all inlet flow rates equals to the outlet flow rates.

It should be pointed out that in the balancing problem the independent variables could be either components of specification vectors (so called state variables)

S_{yx}; $x, y \in \mathscr{K}$ and/or their linear combination (*e.g.* concentration of balanced components in the stream).

For a more generally stated problem the so called controlled simulation Vašek[11] uses the term balancing-simulation. The problem rests again in the determination of the set $\mathscr{Y}_i$, $i \in \mathscr{K}$ whereas the mathematical models of all process units are given (the set of transformation $\mathscr{F}$), however, the independent variables can be some parameters of the process units – elements of the set $\mathscr{D}$, as well as the state variables and their functional dependences. (In both last mentioned problems the selection of the independent variables must be made so that the solution of the problem is unique).

While the "purely" balancing problem is solved mostly by a different type of programs *e.g.* SYMBOL[12], BILL[13], DEBIL[14], the simulation programs (Table I) are used for solution of the open simulation and some – though in a limited range – of balancing–simulation problems. The balancing-simulation problem (also callled the controlled simulation) appears very frequently in the design calculations. However, its general solution is usually more difficult than the solution of the open simulation problem as well as its specification having a unique solution. Sometimes it is also possible to use for balancing-simulation problem solution the programming system which operates in the performance mode so that a number of open simulation calculations is run while the design parameters of the process units are varied, *e.g.* heuristically, so long until the specified value is reached. Some of the programs for simulation of chemical processes are furnished with some additional mathematical models of process units which allow one to use them not only in the performance mode but also in the design mode. As an example the heat exchanger with the given temperature of one of the outlet streams may be quoted. An intensive research has been made in this field recently – one of way out being the extension and modification of existing simulation programs (Vašek and coworkers[15]).

Basic Modules and Structure of Flowsheet Simulation Programs

An excellent analysis of the basic structure of simulation programming systems has been given by Evans, Steward and Sprague[16]. They recognize three basic parts: *1*) Representation of the problem within the computer, the program and data structure; *2*) the mathematical solution of the problem, computational techniques; *3*) communication between the user and the system, the input and output parts.

Thus specified structure is mostly realized by modules (programs or procedures) mutually interconnected so that they form the programming system (an example of a structure is indicated in Fig. 2).

Survey and Classification of Selected Programming Systems

From the beginning of the sixties a number of general-purpose simulation systems has been developed. Let us make an attempt to survey at least the several best known or the most interesting programming systems and to evaluate them critically particularly to review their strong points. The information obtained may be used then for prediction of the present trend in their development.

Similar investigation have been published in recent years by various authors – a survey of the period up to the year 1968 was given by the mentioned Evans, Steward and Sprague[16], for the period 1968–1971 by Flower and Whitehead[17,18]. Surveys are also given by Sargent[19,20], Umeda[21] (unfortunately the largest part of his study is in Japanese), Gruhn, Dietzch and Reiner[22], Kehat and Shacham[3,23,24]. A comparison of some system has been published by Peters and Barker[25], Balls and coworkers[26].

Some more detail information on 14 chemical engineering simulation systems is given in Table I. There are also incorporated two balancing programs (DEBIL and

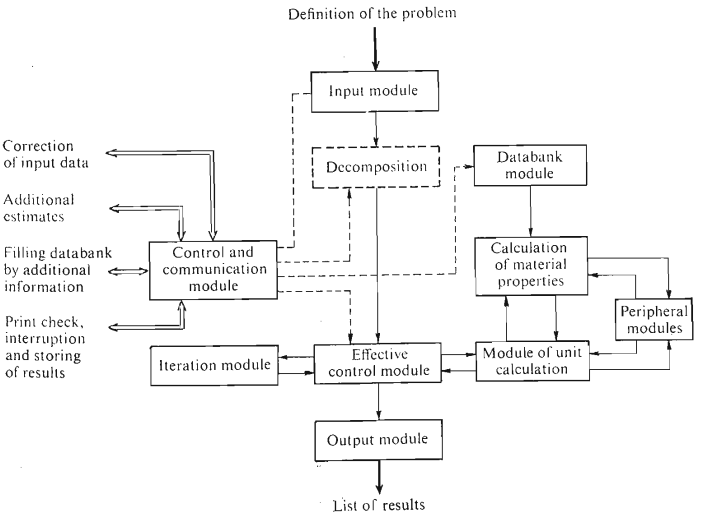

Fig. 2
Example of Structure of Simulation Programming System

TABLE I

Survey of Chemical-Engineering Simulation Systems

Name of system	Authors organisation year of completion described version	Purpose	Language; computer; request core storage (bytes)	Basic: input mode	Basic: thermodynamic and physical data bank
DEBIL (Design balancing module)	VÚCHZ Brno 1973	balancing	ALGOL 60; ODRA 1204; 16 K	input language	—
BILL and supporting programs	VŠCHT Praha 1973	balancing, choice of the balance measurements, smoothing of measured values	FORTRAN; IBM 360, 370 TESLA 200; 100 K	—	—
SIPRO version 74 (Simulation programming system)	VÚCHZ Brno and VUT Brno 1974	steady state simulation	ALGOL-GENIUS; DATASAAB D 21; 30 K words	input language; 54 indicated errors	54 components
GOLEM (Generally oriented language for energy and material balance)	CHEMOPROJEKT Praha 1973	steady state simulation	PL/I; IBM 360/40; 52 K	none	5 components
SIMUL	Chemical trust Budapest 1970	steady state simulation, optimization	ALGOL 60; GIER; 1 K words	input language	210 components
RSS-2 (Raschot slozhnykh skem)	NIFCHI Moscow (VEB PK Schwedt) 1972	steady state simulation	ALGOL 60; MINSK 22; 7 K words	none	
SYSCOM	VEB Petrochemisches Kombinat Schwedt, GDR 1973 (Nifchi Moscow)	steady state simulation and optimization	ALGOL; NE 4130;	indication of errors	?
CONCEPT Mark 3 (Computation on-line of networks of chem.-eng. process technology)	CAD Centre Cambridge, 1973	steady state simulation and economic evaluation	FORTRAN; IBM 370/125; UNIVAC 1108; ATLAS; virtual memory	conversation interactive language, partial indication of errors	105 components

TABLE I
(*Continued*)

modules					
method of calculation of vapour–liquid equilibria and enthalpies	decomposition	method of solution of non-linear or differential equations, convergence acceleration	library of models (unit calculations)	Application	Ref.
—	reduction of the balance scheme	—	—	balancing of sugar refineries oil dewaxing plant	14, 27
—	reduction of the balance scheme	—	—	adsorption column reactor NH_3 electrolyses NaCl pyrolysis	13, 28, 29, 30, 31, 32, 33
Antoine, Chao-Seader, Grayson-Streed; Redlich-Kwong, Edmister	recycle loops location, determination of the calculation sequence	simultaneous, sequential-simple repeated substitution, -approximation with relaxation	42 models	hydrogenation heat exchanger train in crude oil distillation unit oil dewaxing plant	10, 34, 35, 36
Chao-Seader, BWR	none	sequential; -simple repeated substitution	14 models	ammonia synthesis production of synthesis gas by reforming	37, 38
Antoine; Redlich-Kwong	none	sequential -modified Newton-Raphson, -relaxation; Runge-Kutta-Merson	20 models	production of ethylene production of acetylene	39, 40, 41, 42, 43, 44
?	recycle loops location, determination of the calculation sequence	sequential, -Wolfe; Runge-Kutta	?	conversion of methane and oxidation of carbon	45, 46, 47
Benedict-Webb-Rubin; Redlich-Kwong	recycle loops location, determination of the solution sequence	sequentia-simple repeated substitution, -Wegstein, -Broyden, -Wolfe, -Powell; Runge-Kutta	20 models	organic synthesis	48, 49, 50
ideal mixture, Chao-Seader; Yen-Alexander	recycle loops location, determination of the calculation sequence	sequential-simple repeated substitution, approximation with relaxation, -geometrical interpolation, -linearisation	40 models	compressor unit of ethylene process	51, 52, 53

TABLE I
(*Continued*)

Name of system	Authors organisation year of completion described version	Purpose	Language; computer; request core storage (bytes)	Basic input mode	Basic thermodynamic and physical data bank
PACER 245 (Process Assembly Case Evaluator Routine)	Digital Systems Corp. Hanover 1971	steady state simulation and economic evaluation, optimization	FORTRAN; CDC 3600, IBM 370; virtual memory	input language, indication of errors	101 components
CHESS (Chemical engineering simulation system)	University of Houston 1971	steady state simulation	FORTRAN; IBM 360, UNIVAC 1108, CDC 6400;	partial indication of errors	98 components
GEMCS (General Engineering Management Computation System)	McMaster University, Hamilton, Ontario and Canadian General Electric Co. Ltd. 1969	steady state simulation	GE Time Sharing FORTRAN; General Electric 265; 5.2 K words	limited conversation	none
GFS (General flowsheeting program)	M. W. Kellog Co.	steady state simulation	FORTRAN; IBM 360/40, IBM 370; 100 K	none	48 components
TISFLO (Technological Information System)	Duch State Mines, Central Laboratory Geleen, Netherlands 1972	steady state simulation, economic evaluation	?	input language, indication of errors	120 components
FLOWPACK (Process Flowsheeting Package)	ICI, Central Instr. Res. Laboratory Runcorn 1970	steady state simulation, economic evaluation	FORTRAN IV; IBM 360, ICL 4; 150 K	input language, indication of errors	65 components
FLOWTRAN (Flowsheet Translator)	Monsanto Enviro — Chem. systems Inc. St. Louis 1972	steady state simulation, economic evaluation	FORTRAN; CDC 6400, 64 K words, IBM 360/50, IBM 370/145, 384 K Honeywell 6080, 64 K words	input language, indication of errors	200 components
CHIPS (Chemical engineering information processing system)	Service Bureau Corporation 1966	steady state simulation	FORTRAN; IBM 7040/44, IBM 7090/94, IBM 360;	?	?

TABLE I
(*Continued*)

modules					
method of calculation of vapour–liquid equilibria and enthalpies	decomposition	method of solution of non-linear or differential equations, convergence acceleration	library of models (unit calculations)	Application	Ref.
Antoine, Chao-Seader, BWR, NRTL, Renon and Prausnitz and other methods	recycle loops location, determination of the calculation sequence	sequential-simple repeated substitution (others can be supplied by the user)	163 models (on different levels simulation and also for economic evaluation)	production of chlorine formaldehyde, sulphuric acid	54, 55
Chao-Seader, Grayson-Streed; Yen and Alexander	none	sequential-simple repeated substitution, -Wegstein	15 models	polymerisation of olephines	56, 57
interpolation from tables, approximation by a polynomial	location max. three recycle loops	sequential-simple repeated substitution,-linear approximation	6 models	sulphuric acid process	58
?	none	sequential-simple repeated substitution	11 models		59
Antoine, Chao-Seader; Maxwell-Lee, Erbar, Edminster	—	simultaneous-sequential	?	polymerization	60, 61
Antoine, Chao-Seader, Wilson	recycle loops location, determination of the sequence of solution (at the request of users)	sequential-simple repeated substitution, -scalar acceleration, -modification of secant methods	18 models	acetic acid	62, 63, 64
Antoine, Chao-Seader, Grayson-Streed, Van Laar, Wilson, NRTL and others	none	sequential-simple repeated substitution-Wegstein	42 models (economic evaluation incorporated)	chlorination of decane	18, 65, 66, 67
?	none	sequential	24 models	purification of crude oil	26, 68, 69, 70

TABLE I
(*Continued*)

Name of system	Authors organisation year of completion described version	Purpose	Language; computer; request core storage (bytes)	Basic input mode	Basic thermodynamic and physical data bank
REMUS (Routine for executive multi-unit simulation)	The University of Pensylvania, 1970	dynamic simultation	FORTRAN; IBM 360, 370	indication of 84 types of errors	—
DYNSYS (Dynamic systems simulator)	McMaster University, Hamilton, Ontario, 1970	dynamic simulation	FORTRAN; IBM 360, 370	none	—

BILL) and two systems for simulation of unsteady states (REMUS and DYNSYS) which, however, are not the subject of our analysis but which are frequently used as modules of computer-aided design systems. Beside those presented in Table I let us list some other systems such as the DIGSIM (Arndt and Langer[74,75]), PGCC (Michelot[76]), PEETPACK (Peters and Barker[77]), GPS (McDonnel Douglas Comp.[78]), DESIGN (Chemshare Corp.[79]).

The first four columns of the Table contain the basic identification characteristics (Name, source, area of application, programming language and the computer on which the system has been implemented). The next six columns are more detailed specification of the individual modules as indicated in Fig. 2 and the last two columns are giving examples of industrial applications and references from which the given information were taken. Apart from the most known simulation systems from the Western countries some systems from Czechoslovakia, Hungary, GDR and USSR have been included, that is those of which a comprehensive review has not yet been published. All given systems are used for modelling of continuous chemical processes. For solution of batch operations the more generally oriented simulation systems can be used such as the GPSS (General Purpose Simulation System[80]) of the IBM Corp. or SIMSCRIPT (Briddell[81]). There were also some special systems particularly designed for simulation of batch processes such as the MULTI-BATCH package (Sparrow and Rippin[82]) which is moreover supplemented with the economic evaluation of the process. A comparatively less attention has been paid to the development of the latter, nevertheless they have for solution of the given problems unquestionable significance.

TABLE I
(Continued)

modules					
method of calculation of vapour–liquid equilibria and enthalpies	decomposition	method of solution of non-linear or differential equations, convergence acceleration	library of models (unit calculations)	Application	Ref.
—	—	16 integration methods	16 models		71
—	—	1 integration method; Adams-Moulton--Shell predictor-corrector	9 models	production of chlorine hydrolysis	72, 73

Development of simulation programs is at present carried out by three types of institutions (Briddell[2]): *a*) Universities, b) Engineering and consulting firms, *c*) Big companies producing chemical equipment or products. Each system is of course affected by its source. Programs from universities mostly concentrate on demonstrations of new mathematical methods or they are used for teaching purposes. They are usually simpler, relatively easy to get but their significance for industrial application is of less importance. Original version of CHESS or GEMCS may be quoted as systems of academic level. In institutions of other two types more complicated and industrially oriented systems are being formed, but it is usually hard to obtain them for an external user. The industrially oriented systems are available in large chemical process companies mostly for their internal use. On the other hand engineering and consulting firms make them available to customers and offer the supporting services, of course on a completely commercial basis. *E.g.* the commercial version of the PACER 245 which is offered by the Digital System Corporation[83] is available for 90000 $, the FLOWPACK for 20000 Lstg (in 1972 prices).

Individual systems thus differ in their generality, complexity and extension as well as by the field of applicability. (The majority of systems cover approximately the same range – refineries, petrochemistry and recently also waste water treatment). It is interesting to note that some of the systems appart from open simulation make it possible to tackle also a limited range of controlled simulation (balancing-simulation) problems and to perform a very important economic evaluation (CONCEPT, PACER 245, FLOWTRAN, TISFLO) or they have buit-in optimization procedures (SIMUL, SYSCOM). Thus they form, in a way an initial stage of integrated com-

puter aided design systems, since both the economic evaluation and optimization is carried out in these programs, however, as separate activity which usually follows the actual simulation and is secured by simple extension by additional modules. Thus essentially only simulation problems can be solved. Although some other systems have a separate module for economic evaluation there still exists a possibility for the close cooperation with the simulation program *i.e.* the more or less integrated approach – SIPRO-ECOS (Dohnal and coworkers[7]), CHESS-CHEEP (Worley and Motard[84]).

At present, the input problem-oriented language together with input data checkins are the standard feature of the majority of simulation systems. The question is hog- a particular language suits the needs of the user. To be able to answer this it is necew sary to test the individual systems in the field application.

The thermodynamic and physical properties data base is also incorporated almost in all systems. The most comprehensive are data banks of SIMUL, FLOWTRAN, TISFLO. Apart from the size of the data base also the selection of components, accuracy and consistency of data are of great importance. These aspects are in some detail considered *e.g.* in the study by Jícha[85].

The methods of thermodynamic and physical properties calculation exhibit very similar features since most of the systems are oriented on petrochemical proces- ses. The usual Antoine equation for vapour–liquid equilibria is mostly complemented by the Chao-Seader or Grayson-Streed correlation. PACER 245, FLOWTRAN and TISFLO offer a wide range of methods to choose from.

The sequential method is used by the majority of systems where beside the simple repeated substitution some means of the convergence acceleration may be included. The question of convergence accelerators usage is still to be answered because in a particular application, however, they might have the detrimental effect upon the convergence, as it is *e.g.* pointed out in the user's manual of CONCEPT[51]. Nearly in all cases it is up to the user to decide which from the offered methods to select. CHESS, GFS, GOLEM and CHIPS do not have the decomposition modu- les; this can be frustrating in solution of more complex processes. Recently, a greater attention is again paid to the simultaneous method (Umeda and Nishio[86], Klemeš and Vašek[10], Kehat and Shacham[87], Futterer and Schlosser[88]) or to its combination with the sequential approach (de Leeuw den Bouter[60], Timar and Pilhofer[89]).

An important indicator of the system applicability is the number of unit operation models in the library. A fairly large library may be found in SIPRO (42 models), PACER 245 (total of 165 models out of which 40 are ment for simulation), CONCEPT (40 model), FLOWTRAN (29 simulation models).

Majority of systems in the western countries is programmed in FORTRAN. This seems to be the result of wide application of IBM computers (FORTRAN has been introduced by IBM). FORTRAN oriented systems have a certain advantage

in unification and in the possibility to use various computers since FORTRAN is relatively independent of the type of computer and is widely implemented.

But FORTRAN also indicates a number of limitations and disadvantages which according to our opinion prevail. The most important one is the impossibility to use dynamic storage allocation which causes on the one hand an ineconomical utilization of the memory while, on the other hand, to an *à priori* limited number of nodes, streams and components in the simulated process (*e.g.* in CHESS – 50, 100, 20 or in CONCEPT – 50, 150, 20). Though these limitations are not, judging superficially, too important we must realize that *e.g.* CHESS cannot solve problems with one node, two streams and 21 components without changing the program coding. Similar limitations also hold for the number of streams incidental with the node. *E.g.* the CHESS allows only 7 incidental streams; this may present some problems if a column with several feeds and sidestreams is a part of the simulated process.

Some other drawbacks of FORTRAN for the use in simulation systems can be mentioned: the more complicated manipulation with the data files and with the non-numerical expressions, the difficult use of the block structure and nonexisting recursive procedures, higher probability of overlooking of faulty implicit declarations.

Some of the quoted problems can be eliminated by use of ALGOL or of the more suitable higher programming languages such as ALGOL-GENIUS (SAAB Co[90]; which is ALGOL complemented by some features of COBOL) or PL/1 (IBM Corp.). It is to be expected that PL/1 will be implemented by makers of larger computers and on unified EC computer series of CMEA countries.

If we finally summarize the evaluated aspects, the 14 simulation systems given in the review can be roughly divided into two groups: *a*) The well-developed systems with the problem-oriented input language and input data checking, having the sufficient data bank and satisfactory methods of thermodynamics and physical properties calculations, with the automatic determination of the calculations sequence with the possibility of the convergence acceleration; having a large library of unit calculations. Such systems are *e.g.* PACER 245, CONCEPT, SIPRO, FLOWPACK, SYSCOM, FLOWTRAN, TISFLO. *b*) Systems in which some parts have been brought to a high standard, however they are in some respect deficient (*e.g.* decomposition, problem-oriented input language, more extensive library of unit calculation is missing).

It should be emphasized, that the above evaluation does not consider the frequency by which the particular system has been industrially applied. (*E.g.* the authors of FLOWTRAN[65] claim that in the period of two years 1972–74 they had from 400 to 1000 applications per month). The comparison of systems has been, moreover, made on basis of the published information only and so it was not possible to assess such important features as the standard of programming and thus ensuing calculation speed, flexibility from the view point of the user *etc.* Certain comparison of these

aspects at least of several systems (PACER 1966 version, GEMCS, CONCEPT) has been given by Peters and Barker[25]. On basis of available information it may be found that some systeme exhibite very good properties of their parts. *E.g.* in CONCEPT it is the input conversation interactive feature and library of models; in PACER 245 the data bank and the whole set of procedures for thermodynamic and physical properties calculation, library of models; in SIPRO the problem-oriented language, possibility of choice of the simulation method and models library; in RSS-2 and SYSCOM decomposition and the convergence acceleration (these modules are similar since they were developed in cooperation); in SIMUL it is the data bank; in FLOWTRAN also the data bank and calculation of properties; in TISFLO the combined simultaneous-sequential simulation method.

In general, a great attention is usually paid to the decomposition module and to the iteration procedures for solution of non-linear equations. But for industrial use other features are also important *i.e.*

- well developed input language, or the conversation interactive approach,
- satisfactory data bank and procedures for properties calculation,
- possibility of simple transaction or addition of modules by the user (*e.g.* calculation of equilibrium, process unit model),
- users specified output format of results,
- easy comprehension of the philosophy and operation rules of the simulation system.

Gruhn, Dietzch and Rainer[22] have summarized the most important requirements on simulation systems as follows: Generality with respect to the problems which are to be solved, as small as possible requirements on the computer technique and as large as possible comfort for the user.

Present Trend and Conclusions for Future Development of Simulation Systems

The number of existing chemical engineering simulation systems is estimated by Winter and cowokers[53] to be more than 60. Villadsen[91] in his review states that he has found 74 references in literature and that this number is not final. He disputes the duplicity of the research and development capacity in this field.

Why such a number of simulation systems is being developed, if one considers that each of them represents the effort of several people for several years.* There are several reasons why this has happened. Let us make an attempt to name just a few: *a*) Large companies try to be independent, the majority has their own calculation methods, mathematical models are essentially the design procedures and thus their

* Monsanto Co notes[65] that the FLOWTRAN has needed approx. 60 man-years and that the cost has exceeded 2·25 milions $.

simulation systems represent important part of their know-how; *b*) some of the published systems are not ready to use and are not completely tested, others are developed only on the academic level; *c*) the purchased simulation programs usually require the service of a rather specialized staff, sometimes also the cooperation of the authors; *d*) the systems core is based on the solution of the set of nonlinear equations; since there does not exist, in general, the best method for their solution, the authors of various programs are using methods which appear to be most advantageous from their point of view; *e*) the considerable and most labourious part of simulation systems are mathematical models of process units, the modules for calculation of thermodynamic and physical properties and the data bank. Each of systems, though basically general, has more perfectly developed those models and procedures which the organization needs most; *f*) though it seems that an enormous effort in preparation of programs is wastefully duplicated this is not quite true. Most of the simulation systems published under a new heading usually utilize some parts of earlier systems provided they are available as a listing and they suit the needs of the programmer. A number of systems are basically applying the structure and executive program of PACER (*e.g.* CHESS, GEMSC, GOLEM, USP[92,93], GEMBV[94]); *g*) if the system is to be used effectively it is absolutely mandatory that a manual of a good quality is at the users disposal so he would know how to prepare new process unit models and other modules to meet his needs. Incorporation of the new modules must be flexible and easy. If this is not the case the user tries to develop his own system; *h*) majority of systems can be implemented on computers of a certain type or series only; *i*) it is difficult to determine the suitable degree of generality; there exist systems which have almost unlimited application, however, based on considerable simplifications and consequently on inaccurate models while on the other hand there are very complex systems oriented only to the specialized class of problems.

The potential user and/or designer of a simulation system should bear in mind the following:

The importance of simulation programs increases with the rising cost and with difficult availability of raw material and energies since this trend leads to the necessity to design more complex equipment which would utilize the raw material more efficiently. They enable the process designers and engineers to pay more attention to the creative work and to spend less effort with tiresome routine calculations.

Simulation systems are also an important modules in developing of integrated computer aided systems. Although it is possible to obtain relatively cheap systems with very simple models on the so-called University level, the industrially applicable systems are rather expensive (*e.g.* the already mentioned PACER 245 costs 90000 $). If an organization decides to buy a simulation system, it is to some advantage to arrange for its maintenance and service should the trouble-free operation be secured.

The lease for a single use is suitable for smaller organizations. The list and basic characteristics of simulation programs which are commercially available is periodically published in Chemical Engineering[55,95–97] (mostly from USA). In Czechoslovakia this practice has been introduced by Chemický průmysl[98]. Provided the lease simulation program is used some problems with data security and confidence may arrise (Seider[99]).

For larger corporations with a certain specialization it is obviously reasonable to develop their own simulation system based on all the available external information or programming modules. A byproduct of design of own simulation system appears to be a thorough training of specialists which are fully capable to take care of the service within the organization.

It would be desirable to conduct the development of a generalized simulation system so this would be capable to integrate into widely accepted structure having the generally accesible and private data bank together with the library of process unit models. The most prominent feature of such a system should be easy and simple modification, complete change and addition of modules with various levels of complexity according to needs of the user.

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