LARGE QUALITATIVE MODELS OF COMPLEX CHEMICAL AND BIOENGINEERING PROCESSES

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Qualitative model is a theoretical background of commonsense. Complex qualitative models can have prohibitively many solutions (qualitative states). Therefore a qualitative analogy of such classical quantitative tools as e.g. the decomposition is developed. Practical applications of decomposition principle is nearly always ad hoc. Therefore two case studies are presented in details, a chemical process (mixer, chemical reactor, separator) and an anaerobic fermentor.

Real engineering systems (e.g. petrochemical process, fermentation, pollution tasks) are complex, integrated, ill known and difficult to measure systems. They may be subject to extremely complex relations with their surroundings which may make it nearly impossible to isolate them without a substantial distortion of the available knowledge. Therefore scientific knowledge of such systems may be inconsistent, sparse, uncertain and represented by different formal tools[1]. In order to model complex systems effectively, all the available information must be used. Even very uncertain knowledge is valuable. It is the effectiveness with which uncertain knowledge is used which is very often the main distinction between good and bad models of the same system. At present, most of the techniques employed for the analysis of complex engineering problems (e.g. bioengineering, environmental control, computer integrated manufacturing, reliability) possess analytical and/or statistical natures. Unfortunately these precise mathematical tools do not always contribute as much as is expected towards a full understanding of engineering tasks.

COMPLEX INDUSTRIAL SYSTEMS

Engineering knowledge represents a heterogeneous complex of various types of knowledge. The following classification is perhaps typical[2,3]:

- deep knowledge (laws of nature)
- equations
- quantitative (i.e. numerical values of constants are known)
- qualitative (i.e. constants are numerically unknown)
- shallow knowledge

– quantitative
– equations (e.g. approximation)
– measurements
– conditional statements
– qualitative
– heuristics (e.g. if pressure goes down then deviation goes up).

The following quantifiers can be used:

– real number
– fuzzy set[4]
– number[5]
– rough set[6]
– verbal specification[7]
– cognitive description[8].

It is usually not difficult to collect some relevant equations which represent several laws of nature to form a nucleus of a classical mathematical model. However to develop a model that reflects essential features of reality is very often time-consuming and expensive.

It can be hardly expected that conventional techniques (analytical and/or statistical) can analyse a real problem entirely. A model description of the object under study must be simplified while working with conventional tools. It is not paradoxical that less information intensive methods of analysis (e.g. fuzzy mathematics, qualitative models – naive physics) achieve more realistic results, provided that the system which is modelled is too complex, and/or ill known.

Commonsense analysis of engineering problems is less than one decade old. In spite of this commonsense models (naive physics qualitative model) offer a very flexible formal tool to deal with realistic engineering tasks. See e.g. refs[1–3].

It is extremely difficult or impossible to solve simulation problem of complex (large) industrial sastems by classical methods (e.g. statistical analysis). When an engineer is asked to explain an operation of the large and complex system he/she will often describe it in terms of a sequence of events each of which is caused by previous events. The key problem is how the system responds to input perturbations such as an increase (decrease) of e.g. flowrates, concentrations and temperatures. Therefore a flexible tool is needed to formalize a large part of ordinary everybody knowledge of the physical word[9]. Such formal tool seems to be naive physics.

A general algorithm which formalizes a commonsense through naive physics does not exist. Perhaps a qualitative model is the best available approach which can be used as a theoretical background for a development of computer programs and consequently of the expert system of the second generation.

However the next generation of expert systems will not be available for routine application too soon. Therefore commonsense approach can only be realized through qualitative models.

QUALITATIVE ALGEBRA

Qualitative model is fairly new. To make this paper self-consistent a semi-intuitive presentation of the basic concepts is given. See e.g. refs[10-12].
In this paper qualitative variables are denoted as

$$X_1, \ldots, X_n \,. \tag{1}$$

Qualitative variables have the following qualitative values

$$(k+, k-, k0)\,, \tag{2}$$

where

$$\begin{aligned} k- &= QR(-\infty, 0) \\ k0 &= QR(0) \\ k+ &= QR(0, \infty) \end{aligned}$$

QR qualitative representation.

The letter k is used to make the clear difference between a set of qualitative values and algebraic operations + and −.
A qualitative dynamic behaviour of a system under study is specified by qualitative derivatives. $\mathrm{D}X_i$ is the first derivative of X_i and $\mathrm{DD}X_i$ is the second derivative.

$$\begin{aligned} \mathrm{D}X_i &= QR(\mathrm{d}X_i/\mathrm{d}t) \quad (\text{see } (2)) \\ \mathrm{DD}X_i &= \mathrm{D}(\mathrm{D}(X_i)) \end{aligned} \tag{3}$$

t time.

Our experience with solutions of different problems (chemical and mechanical engineering, bioengineering etc.) shows that it is sufficient to consider the following qualitative specification of variable X_i

$$(X_i, \mathrm{D}X_i, \mathrm{DD}X_i)\,. \tag{4}$$

There are n qualitative variables in the model (see (1)). Therefore n-triplets must be used to specify a dynamic behaviour of the system i.e. a set of qualitative states. The j-th qualitative state is

$$(j, (X_1, \mathrm{D}X_1, \mathrm{DD}X_1), \ldots, (X_n, \mathrm{D}X_n, \mathrm{DD}X_n)) \quad j = 1, 2, \ldots, z\,, \tag{5}$$

The n-triplet (5) is a qualitative state.

Qualitative Operations

Any qualitative operation is fully specified if an algorithm how to evaluate its triplet (*4*) is given. The following qualitative operations are considered in this paper: addition, multiplication, time derivative and parametric derivative.

A qualitative addition is

$$X_i + X_j = X_s \tag{6}$$

$$\begin{array}{cc|ccc} & & & X_j & \\ & & k+ & k0 & k- \\ \hline & k+ & k+ & k+ & ? \\ X_i & k0 & k+ & k0 & k- \\ & k- & ? & k- & k- \end{array}$$

where z is the total number of qualitative states.

The question mark (see (*6*)) indicates conditions under which it is impossible to predict a sign of the result:

$$(k+) + (k-) = ?\ . \tag{7}$$

Therefore a qualitative model of an engineering problem with many additions may generate prohibitively many qualitative states.

A qualitative multiplication is

$$X_i * X_j = X_s\ . \tag{8}$$

Its matrix is so transparent that is not given here.

A qualitative time derivative is simple. If qualitative variable X_i is a derivative of variable X_j then:

$$\begin{aligned} X_i &= \mathrm{D}X_j \\ \mathrm{D}X_i &= \mathrm{DD}X_j \\ \mathrm{DD}X_i &= \mathrm{DDD}X_j\ . \end{aligned} \tag{9}$$

A time derivative (*9*) does not cover all requirements of practical applications. A parametric derivative is needed. The parametric derivative is

$$\mathrm{D}X_i/\mathrm{D}X_j \tag{10}$$

$$\mathrm{DD}X_i/\mathrm{DD}X_j\ . \tag{11}$$

This parametric derivative is very useful e.g. for qualitative description of e.g. control loops. It represents a qualitative description of a relation between two variables. For details see refs[11,12].

QUALITATIVE MODEL

Qualitative model S_M i.e. a set of qualitative relations can be divided into two submodels. The first submodel M_D is a set of such qualitative equations that are induced by laws of nature. They usually represent deep knowledge. M_S is a set of qualitative relations based on shallow knowledge.

$$S_M = S_{MD} \cup S_{MS}$$
$$S_M \cap S_{MS} = \varnothing$$

The characteristic feature of both submodels M_D and M_S is that they represent general knowledge. A specific point of view represents qualitative question Q. The question Q is mostly a set of qualitative assignments

$$\begin{gathered} X_i \leftarrow T_1 \\ DX_i \leftarrow T_2 \\ DDX_i \leftarrow T_3 \\ T_1, T_2, T_3 \in (k+, k0, k-)\,. \end{gathered} \tag{12}$$

A qualitative solution of a qualitative model S_M (without any additional question Q) is set M of n-triplets (5) which are qualitatively correct (i.e. they "agree" with all equations of model S_M.

The set of qualitative states (solutions (see (5)) represents a general knowledge of a problem under study. Any additional constraints eliminate some elements of M. It is clear that e.g.

$$s_Q \subset M\,,$$

where s_Q is a set of qualitative solutions of the following model:

$$S_M \cap Q\,, \tag{13}$$

where Q is a set of the assignments (12).

The n-triplet (5) belongs to the set of solutions of model S_M, ($M \cap Q$ etc.) if it is not rejected by any model relation.

LARGE QUALITATIVE SYSTEMS

A large qualitative system (LQS) is a system which cannot be solved without a decomposition. The number of LQS variables (see n in (5)) is rather vague. It depends heavily on an available computer hardware. Perhaps 30 variables is a limit for personal computers.

A realistic industrial system (e.g. petrochemical process) can have more than 5 000 variables. The total number of the qualitative states (*5*) can be (expert estimation) more than 10^{10}. Therefore a certain form of decomposition is needed.

Some engineering systems (e.g. chemical, food and pharmaceutical technologies) can be decomposed into special classes of subsystems. These sub systems are mostly typical pieces of equipment (e.g. heat exchanger, turbine, batch fermentor). A concept of unit operation (for details see e.g. refs[13,14] was developed to minimize an extent of theoretical and experimental work which is needed to develop classical mathematical model of complex engineering system.

To avoid a very expensive development of formal qualitative models of these typical subsystems usually a submodel library is used. For details see e.g. SPEED UP system[15].

A solution of any qualitative model is a discrete set because of discrete nature of qualitative variables (see (*2*)). A solution can always be presented in a form of a matrix where the i-th solution (*5*) is the i-th matrix row.

In this case a simulation of the complex system means an integration of pre-solved qualitative models of subsystems. Therefore the library of qualitative models can contain not only qualitative model but even their solutions.

QUALITATIVE INDEPENDENCE

The qualitative models are based on qualitative knowledge QLK. A primitive commonsense analysis confirms that

$$\text{“QLK} < \text{QNK”}\,, \tag{14}$$

where QNK is a quantitative knowledge. The inequality (*14*) means e.g. that $k+$ (see (*2*)) is less information intensive than any positive real number. It is the greatest advantage of a qualitative value. However, it is always less accurate then any real number.

There are two consequences of the inequality (*14*), namely the large number of qualitative states and qualitative independence of some sub systems of the qualitative model.

Every qualitative variable is specified as the n-triplet (*5*). Therefore three parameters are needed to describe completely one qualitative variable.

It is possible that e.g. the second qualitative derivative of i-th variable is totally independent. It means that

$$\mathrm{DD}X_i \in S_j\,, \tag{15}$$

where S_j is the j-th independent sub system. If the second derivative of X_i is the only parameter of the j-th totally independent subsystem S_j, then the cardinality of S_j is equal to one.

Let

$$w(S_j) \tag{16}$$

is the set of parameters of the j-th subsystem. The total number of these subsystems is v

$$S_1, \ldots, S_v . \tag{17}$$

The total number of all parameters is

$$\text{car}\,(W(S_1) + \text{car}\,(W(S) + \ldots + \text{car}\,(W(S_v) = 3n\,, \quad \text{see}\,(1)\,.$$

Example

A simple example is used as an illustrative example. The following equation is a model of undamped oscillation

$$\mathrm{d}X/\mathrm{d}t = -(k+)\,.\,X\,. \tag{18}$$

A positive multiplicative constant can be ignored

$$\mathrm{D}(X) = -X\,. \tag{19}$$

The qualitative model (*19*) has 9 different qualitative states (*5*) as a set of solutions (see Table I). The first variable is a distance, the second is a velocity and the third is an acceleration:

$$X_1 \text{ position}\,, \quad X_2 \text{ velocity}\,, \quad X_3 \text{ acceleration}\,.$$

The result of independence study detects that there are two independent subsystems ($v = 2$, see (*17*))

$$\begin{aligned} S_1 &= (X_1, \mathrm{DD}X_1, \mathrm{D}X_2, X_3, \mathrm{DD}X_3) \\ S_2 &= (\mathrm{D}X_1, X_2, \mathrm{DD}X_2, \mathrm{D}X_3)\,. \end{aligned} \tag{21}$$

The specific deep knowledge of elementary mechanics gives e.g. (see (*20*))

$$\mathrm{D}(\text{velocity}) = \mathrm{D}(X_2) = X_3 \tag{22}$$

It enables us to simplify sets S_1, S_2, see (*21*), as S_1: $\mathrm{DD}X_1 = X_3$, $\mathrm{D}X_2 = X_3$, therefore $(X_1, \mathrm{DD}X_1, \mathrm{D}X_2, X_3, \mathrm{DD}X_3) \rightarrow (X_1, X_3, \mathrm{DD}X_3)$. At the same manner

S_2: $DX_1 = X_2$, $DDX_2 = DX_3$, therefore

$$(DX_1, X_2, DDX_2, DX_3) \rightarrow (X_2, DX_3)\,. \tag{23}$$

The qualitative independence results (*21*) can be rewritten:

Variable	Parameters		
	value	derivatives	
		1st	2nd
X_1 position	S_1	S_2	S_1
X_2 velocity	S_1	S_2	S_1
X_3 acceleration	S_1	S_2	S_1

(*24*)

The independence concept implies a decomposition. It is reasonable to follow this decomposition because the subsystems are mutually independent.

Qualitative Projection

A very simple way how to decrease the solution dimensionality z (see (*5*)) is a qualitative projection. A qualitative n-dimensional space (see (*1*)) is "divided" into two disjoint subspaces i and u. A set of variables I and U can, from engineering point of view, represent a set of interesting I and uninteresting U variables.

Table I

List of all qualitative states of the undamped oscillation (see (*19*))

Solution No.	Position			Velocity			Acceleration		
	X	DX	DDX	X	DX	DDX	X	DX	DDX
1	−	−	+	−	+	+	+	+	−
2	−	0	+	0	+	0	+	0	−
3	−	+	+	+	+	−	+	−	−
4	0	−	0	−	0	+	0	+	0
5	0	0	0	0	0	0	0	0	0
6	0	+	0	+	0	−	0	−	0
7	+	−	−	−	−	+	−	+	+
8	+	0	−	0	−	0	−	0	+
9	+	+	−	+	−	−	−	−	+

Some of the qualitative variables are interesting variables and the rest of variables is considered as non interesting. X is a set of all qualitative variables (*1*):

$$X = I \cup N$$
$$I \cap N = \varnothing\ , \qquad (25)$$

where I is a set of interesting variables and N is a set of non-interesting variables. Provided that variable X_3 is considered as non-interesting then the solutions 1 and 2 are identical.

Solution	X_1	X_2	X_3
1	$(+, +, +)$	$(+, +, +)$	$(+, +, +)$
2	$(+, +, +)$	$(+, +, +)$	$(+, +, 0)$
3	$(+, +, +)$	$(+, +, -)$	$(+, +, +)$

(*26*)

An engineer can study different aspects of his/her problem by a proper choice of interesting and non-interesting variables. It is a sort of a qualitative projection and represents a decomposition (certain point of view).

DECOMPOSITION

Decomposition algorithms as they are used in optimization or conventional flowsheeting (solution of large nonlinear sets of equations) are ad hoc procedures. They are developed for decomposing a problem with specific features. These features are used through a set of heuristics. A similar set of heuristics is not available for qualitative equations.

A simple and powerful heuristics which can be recommended for qualitative systems (especially for qualitative flowsheeting) is decomposition according independent subsystems (see (*17*)). Provided a separate subsystem is too large again, in this case it is recommended to follow a common sense. This approach is used in the case studies.

QUALITATIVE SENECA

A problem of qualitative simulation is very time-consuming and tedious. There are usually many errors provided qualitative problems are solved by hand. Q SENECA (Qualitative SENsible Exper CAtalogue) is an expert system capable of a qualitative analysis. The detailed specification of this system is given in ref.[16], a sufficient theoretical background is given in ref.[17]. What follows is a description of those facts that are needed to understand the bellow given case studies.

A qualitative problem must be described by the following blocks (operations) only:

identification	symbol	description	
$M1$		$DX_j/DX_i = k+$	
$M2$		$DX_j/DX_i = k-$	
$M3$		$M1$ and ($X_i = 0$ and $X_j = 0$)	
$M4$		$M2$ and ($X_i = 0$ and $X_j = 0$)	
$M5$	D	derivative, see (*9*)	(*27*)
$M6$	+	addition, see (*6*)	
$M7$	*	multiplication, see (*8*)	
$M11$		$X_j < X_i$	
$M12$		$DX_j < DX_i$	
$M13$		$DDX_j < DDX_i$	
$M21 - M38$		parametric derivative, see (*10*)	

The qualitative problem is represented by a graph. Every node of this graph is a block (see (*28*)). An arc is a qualitative variable.

QUALITATIVE FLOWSHEETING

Conventional i.e. numerical flowsheeting has been studied for more than 20 years. The advantages and disadvantages are well known. Elimination of some disadvantages requires an introduction some new calculi into flowsheeting. One of them is fuzzy mathematics. See ref.[18].

However it is not enough. A spectrum of various flowsheeting calculi must cover a qualitative flowsheeting as well. The main reason is that the qualitative flowsheeting is a generator of "variants"[12].

Many engineering systems can be decomposed into such subsystems which exchange only energy and/or mass (components). A flowsheet is a special two level hierarchic system. The first level is represented by subsystems (unit operations, see refs[13,14]). The second level is represented by balancing algorithm (mass and energy law of conservation). It "coordinates" the exchange of mass and energy among the subsystems. See e.g. ref.[15].

A system is decomposed into a set of k subsystems

$$R_1, R_2, \ldots, R_k \,. \tag{28}$$

A topology of the system is given by an oriented graph. The set of its nodes is a set of k subsystems (*29*). An arc represents an oriented flow of energy and/or mass. A mass flow is represented by flowates of c components (e.g. oxygen, water).

Let l is a set of component flowrates and enthalpy flux in all streams. A variable

$$l_{i,j,t} \qquad (29)$$

denotes an element of the set l and represents a flowrate of the t-th component in the stream outgoing from a node i and entering a node j.

Further we introduce quantities q which are functions of elements of l only. That is

$$q = q(l) \qquad (30)$$

and

$$s_q \subseteq q\,, \qquad (31)$$

where S_Q is a set formed from elements of q such as component concentrations, specific enthalpy, total flowrate etc.

Let us define a set b so

$$b = q \cup l \qquad (32)$$

that is all its elements are related to balance quantities and determine state of the process; thus they are state variables.

We can now extract some elements from the set l in such a way that a set x_i are those of inputs into the node i (i.e. subsystem R_i) and y_i are those of effluents from node i. Behaviour of a process unit i in steady state is further given by a set p_i of process unit variables. A node i mathematical model is

$$y_i = A[i]\,(x_i, p_i)\,. \qquad (33)$$

A mathematical model of the whole process (system) if formed by two distinct sets of equations. The first set of equations is represented by equations the mathematical models of all subsystems (process units), see (*34*)

$$A = \cup\, A[i] \quad i \in k\,, \qquad (34)$$

where K is a set of nodes (*29*). It should be pointed out, that a mathematical mode equation set $A[i]$ which refers to a subsystem i is usually separable into two groups; one of which expresses the mass and energy conservation law – here denoted $A_C[i]$ and the other represents the engineering rate equations (incorporating the usual transport properties) and is a set $A_R[i]$.

Again for the whole process it is

$$A_C = \cup\, A_C[i] \quad i \in k \qquad (35)$$

and

$$A_R = \cup A_R[i] \quad i \in k \,. \tag{36}$$

The second set of equations t determines a system topology. By this way we simply describe the fact that most of the streams $l_{i,j,t}$ are for some nodes inputs and at the same time for the others outputs; thus

$$s_{i,j,t} \in x_j \tag{37}$$

and also

$$s_{i,j,t} \in y_i \,. \tag{38}$$

Therefore a mathematical model of the whole system (process) is given by an equation set m

$$m = A \cup t \,. \tag{39}$$

The above given definitions enable to describe some specific tasks, namely balancing, simulation and balance simulation.

If a balancing problem is to be solved, the following equations set

$$A_C \cup t \tag{40}$$

has to be satisfied. The independent variables are some elements form the set b (see (*33*)).

In the process simulation, one has to solve the set of equations m while all process unit variables – the complete set p – are given together with limited number of elements from the set L which are selected according to the degrees of freedom rules. The most practical problem seem to be the balance simulation specification. In this case the independent variables may be selected from the sets l, g and p to suit the design purposes best. If we denote the subsets of independent variables (some of their elements are design variables) as l_D, g_D and p_D then the remaining elements – the dependent variables are from the subsets

$$l_C = l - l_D \,, \quad g_C = g - g_D \,, \quad p_C - p - p_D \tag{41}$$

may be found by solving the set of equations m (40).

In principle there are qualitative analogies of conventional algorithms which are used to solve flowsheeting problems. For details see e.g. ref.[18].

CASE STUDIES

Two case studies are presented. The first one is a qualitative analysis of a loop made up by a mixer, chemical reactor and separator. The second case study is a realistic qualitative analysis of a anaerobic fermentor.
To make clear distinction between quantitative and qualitative variables the following indexations are introduced. The case study *Chemical Process* gives all qualitative variables as variables where indexes are in round brackets. The case study *Fermentor* indicates all qualitative variables as variables where X_i is given as Xi.

CHEMICAL PROCESS

A typical chemical process is studied (see Fig. 1). The key part of this process is a chemical reactor. The rest of the process is represented by two sub systems namely a raw material sub system (mixer) and a product purification (splitter).

PROCESS DESCRIPTION

The following notation is used
A concentration of component A, B concentration of component B, F stream flowrate, T temperature, V volume, C temperature of cooling stream, k reaction velocity, Q qualitative constant, t time.
Bracket indexes (see Fig. 1):
re recycle stream, r reactor, si system input, so system output, c cooling, i reactor input, o reactor output.

The above given indexes are used in bracket to emphasize that they are indexes of qualitative vaiables. Dimensions are not given. From the qualitative point of view they are not important. Equally unimportant are multiplicative constants.
The node No. 1 is mixer (see Fig. 1). The law of mass conservation is the only knowledge:

$$F(\mathrm{i}) = F(\mathrm{si}) + F(\mathrm{re}) \tag{42}$$

$$F(\mathrm{i}) \,.\, A(\mathrm{i}) = F(\mathrm{si}) \,.\, A(\mathrm{si}) + F(\mathrm{re}) \,.\, A(\mathrm{re}) \tag{43}$$

$$F(\mathrm{i}) \,.\, B(\mathrm{i}) = F(\mathrm{si}) \,.\, B(\mathrm{si}) + F(\mathrm{re}) \,.\, B(\mathrm{re}) \tag{44}$$

$$Q(\mathrm{i}) \,.\, F(\mathrm{i}) \,.\, T(\mathrm{i}) = Q(\mathrm{si}) \,.\, F(\mathrm{si}) \,.\, T(\mathrm{si}) + Q(\mathrm{r}) \,.\, F(\mathrm{re}) \,.\, T(\mathrm{re}) \,. \tag{45}$$

The Eqs (*43*)–(*46*) are qualitative balance equations (see A_C (*36*)).
A simple chemical engineering analysis of the qualitative constants Q detects simplification. E.g. a specific enthalpy is not a function of temperature. All Q constants are positive. Therefore Eq. (*46*) gives

$$F(\mathrm{i}) \,.\, T(\mathrm{i}) = F(\mathrm{si}) \,.\, T(\mathrm{si}) + F(\mathrm{r}) \,.\, T(\mathrm{r}) \,. \tag{46}$$

The most sophisticated node is the node 2 (Fig. 1). It is given in details in Fig. 2. The following chemical reaction takes place

$$A \rightarrow B \,. \tag{A}$$

Several simplifications are used as e.g. the cooling medium volume is constant, the reactor volume is ideally mixed etc. The consequences can be easily seen from the following equations (see refs[19,20]):

$$\mathrm{d}V(R)/\mathrm{d}t = F(\mathrm{i}) - F(\mathrm{o}) \tag{47}$$

$$\mathrm{d}(V(R) \,.\, A(\mathrm{o}))/\mathrm{d}t = F(\mathrm{i}) \,.\, A(\mathrm{i}) - F(\mathrm{o}) \,.\, A(\mathrm{o}) - V(R) \,.\, k \,.\, A(\mathrm{o}) \tag{48}$$

$$\mathrm{d}(V(R) \,.\, T(R))/\mathrm{d}t = F(\mathrm{i}) \,.\, T(\mathrm{i}) - F(\mathrm{o}) \,.\, T(\mathrm{o}) - Q(1) \,.\, V(R) \,.\, k \,.\, A(\mathrm{o}) - \\ - Q(2) \,,\, (T(R) - C(\mathrm{o}) \tag{49}$$

$$\mathrm{d}(C(\mathrm{o})/\mathrm{d}t = Q(3) \,.\, (C(0) - C(\mathrm{i})) + Q(4) \,.\, (T(R) - C(0)) \,. \tag{50}$$

A correlation between reaction velocity k and reactor temperature $T(R)$ is specified by the M block (see (*28*)), see Fig. 3*a*.

$$k - M27 - T(R) \tag{51}$$

The chemical reactor has two control loops (see Fig. 2). The first control loop (see L_1, Fig. 2) represents a proportional control between flowarate of cooler medium $F(\mathrm{c})$ and the reactor temperature $T(R)$. The second control loop (see L_2, Fig. 2) relates

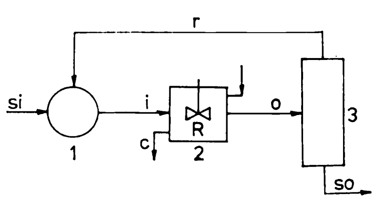

FIG. 1

Flowsheet of a chemical process, 1 mixer, 2 chemical reactor, 3 splitter

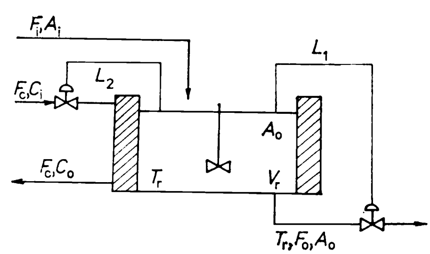

FIG. 2

Chemical reactor and two control loops L_1 and L_2

the pair of variable $F(\mathrm{o})$ and $V(R)$ through proportional control as well (see Fig. 3c). Therefore the following qualitative equations

$$F(\mathrm{c}) - M22 - T(R) \tag{52}$$

$$F(\mathrm{o}) - M28 - V(R)$$

must be considered as a part of qualitative model. This part of the model is not based on any equation.

The node 3 (see Fig. 1) is a splitter:

deep knowledge

$$F(\mathrm{o}) = F(\mathrm{r}) + F(\mathrm{so}) \tag{53}$$

$$F(\mathrm{o}) \,.\, A(\mathrm{o}) = F(\mathrm{re}) \,.\, A(\mathrm{re}) + F(\mathrm{so}) \,.\, A(\mathrm{so}) \tag{54}$$

$$F(\mathrm{o}) \,.\, B(\mathrm{o}) = F(\mathrm{re}) \,.\, B(\mathrm{re}) + F(\mathrm{so}) \,.\, B(\mathrm{so}) \tag{55}$$

$$F(\mathrm{r}) \,.\, T(\mathrm{r}) + F(\mathrm{so}) \,.\, T(\mathrm{so}) = F(\mathrm{o}) \,.\, T(\mathrm{o}) + QQ \tag{56}$$

where QQ is a heat input

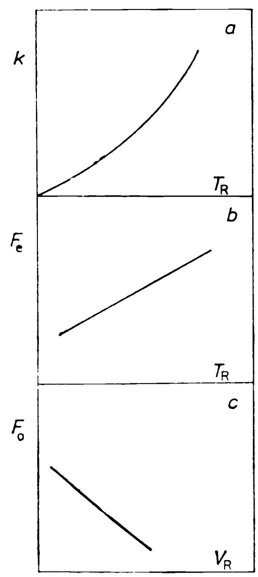

FIG. 3
Graphic representation of shallow qualitative knowledge

shallow knowledge

$$DB(\mathrm{re}) = -DF(\mathrm{re}) \tag{57}$$

$$DA(\mathrm{re}) = DF(\mathrm{re}) \tag{58}$$

$$DT(\mathrm{o}) = -DQQ \tag{59}$$

$$DF(\mathrm{o}) = DF(\mathrm{re}) \tag{60}$$

$$DDF(\mathrm{o}) = DDF(\mathrm{re}) \tag{61}$$

$$DT(\mathrm{o}) = DT(\mathrm{re}) \tag{62}$$

$$D(F(\mathrm{re}) \, . \, T(\mathrm{re})) < D(F(\mathrm{o}) \, . \, T(\mathrm{o})) \tag{63}$$

$$D(T(\mathrm{so}) \, . \, F(\mathrm{so}) < D(F(\mathrm{re}) \, . \, DT(\mathrm{re})) \tag{64}$$

$$DF(\mathrm{o}) < DF(\mathrm{so}) \tag{65}$$

$$DDF(\mathrm{o}) < DDF(\mathrm{so}) \tag{66}$$

The equations (*54*)–(*67*) represent a qualitative subsystem model (*34*).
General deep knowledge is

$$A + B = 1 \, . \tag{67}$$

This equation can be generally transferred into

$$DA = -DB \tag{68}$$

$$DDA = -DDB \, .$$

The qualitative differential equations (*69*) are valid for all streams. It represents the fact that A and B are concentrations.
The values of A and B are always non negative. Therefore a qualitative interpretation of the equation (*68*)

$$A + B = k+ \tag{69}$$

does not represent any additional information.

Decomposition

The system in Fig. 1 is relatively simple. However the total number z of qualitative solutions (see (*5*)) can be prohibitively large. A two level hierarchic approach is chosen to demonstrate how to proceed in such a case.
The most complicated sub system is the chemical reactor. Therefore the chemical reactor is studied separately. This is the first level of qualitative simulation.

The models of the mixer and the splitter are relatively simple. There is no need to study them separately.

Reactor analysis. In order to modify the equations (48)–(53) into a form which is needed for Q SENECA the following variables are used

$$\begin{array}{lll} V(1) = A(\mathrm{o}) & V(5) = F(\mathrm{i}) & V(9) \ = F(\mathrm{c}) \\ V(2) = T(\mathrm{r}) & V(6) = A(\mathrm{i}) & V(10) = C(\mathrm{o}) \\ V(3) = V(\mathrm{r}) & V(7) = T(\mathrm{i}) & V(11) = k \\ V(4) = F(\mathrm{o}) & V(8) = C(\mathrm{i}) & \end{array} \tag{70}$$

The total number of variables is 31. However the variables $X(12)-X(31)$ are auxiliary variables as e.g.

$$X(12) = \mathrm{D}X(3) \tag{71}$$

The Fig. 4 is an example of a graphic representation of the equation (*48*).
A complete specification of the qualitative reactor model is given in Table II. The first line of the second table gives the Eq. (*72*).

Qualitative Independence

The complete description of qualitative independence of the chemical reactor is given in Table III. The first line of this table is (see (*16*))

$$\begin{aligned} X_1 &\in S_1 \\ \mathrm{D}X_1 &\in S_2 \\ \mathrm{DD}X_1 &\in S_3 \,. \end{aligned} \tag{72}$$

There are $v = 13$ (see (*17*)) independent subsystems S. The second subsystem has 81 parameters. It means that number 2 is given in Table III 81 times. All others subsystems have one parameter each. Cardinality of S_1 is one. Therefore the value X_1 is not influenced by any other parameter. It cannot be changed by any other parameter. It is absolutely independent.

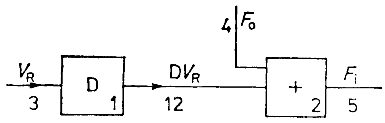

FIG. 4
Graphic description of the equation (*48*)

TABLE II
Qualitative model of the chemical reactor (see Fig. 2)

Block	Operation[a]	Variables	Block	Operation[a]	Variables
1	D	3, 12	14	+	21, 22, 23
2	+	4, 12, 5	15	+	2, 23, 24
3	*	1, 3, 13	16	+	10, 31, 24
4	+	13, 14	17	*	5, 7, 25
5	*	1, 4, 15	18	+	17, 25, 31
6	*	3, 11, 16	19	D	10,26
7	*	1, 16, 17	20	*	9, 10, 27
8	+	14, 15, 19	21	+	26, 27, 28
9	+	17, 19, 18	22	+	10, 28, 29
10	*	5, 6, 18	23	+	2, 30, 29
11	*	2, 3, 20	24	*	8, 9, 30
12	D	20, 21	25	*M*27	2, 11 see Fig. 3*a*
13	*	2, 4, 22	26	*M*22	2, 9 see Fig. 3*b*
			27	*M*28	3, 4 see Fig. 3*c*

[a] See (*27*).

TABLE III
Results of decomposition study of chemical reactor (see (*17*), Table II)

Variable	Parameter			Variable	Parameter		
	X	DX	DDX		X	DX	DDX
1	1	2	3	11	2	2	2
2	2	2	2	12	2	2	2
3	2	2	2	13	10	2	2
4	2	2	2	14	2	2	2
5	2	2	2	15	2	2	2
6	4	2	5	16	11	2	12
7	6	2	7	17	2	2	2
8	8	2	9	18	2	2	2
9	2	2	2	19	2	2	2
10	2	2	2	20	13	2	2
				21–31	2	2	2

Man-Machine Dialogue

One qualitative question is specified by Table IV. E.g. the third row of the Table IV gives the reactor volume specification.
The value of the liquid in the chemical reactor is positive (i.e. the reactor is not empty). The first qualitative derivative is positive, i.e. the reactor volume goes up. The second derivative is not specified. A question mark? indicates that a certain value is not specified as apart of the question.
The expert system Q SENECA indicates inconsistencies (see Tables III and IV) in the specification of the reactor temperature $T(R)$ and the flowrates of the cooling medium $F(\mathrm{c})$. $F(\mathrm{c})$ does not correspond to the Eq. (*53*).
Table IV gives

$$\mathrm{D}T(R) = +$$

$$\mathrm{D}F(c) = - \,.$$

Block (*53*), the block No. 26 in Table III

$$\mathrm{D}T(R) = \mathrm{D}F(\mathrm{c})\,.$$

Therefore as a part of a man-machine dialogue the question (i.e. Table IV) must be modified. Let us suppose that the $F(\mathrm{c})$ i.e. $V(9)$ (see (*71*)) is modified as follows

$$(+, +, +) \quad \text{or} \quad (?, ?, ?)\,.$$

The answer obtained by Q SENECA is

A(o)			V(r)			F(o)			C(o)		
X	DX	DDX	X	DX	DDX	X	DX	DDX	X	DX	DDX
+	?	?	+	+	−	+	+	−	+	?	?

TABLE IV
Qualitative question that is solved together with the reactor model (see Table II)

Var.	No.	X	DX	DDX	Var.	No.	X	DX	DDX
A(o)	1	+	?	?	A(i)	6	+	0	0
T(R)	2	+	+	+	T(i)	7	+	+	−
V(R)	3	+	+	?	C(i)	8	+	0	0
F(o)	4	+	?	?	F(c)	9	+	−	?
F(i)	5	+	−	−	C(o)	10	+	?	?

where

$$? = + \quad \text{or} \quad 0 \quad \text{or} \quad - \,. \tag{74}$$

The solution (*74*) together with the question (see Table IV) qualitatively specifies all variables $V(1)-V(10)$, see (*71*).

The solution (*74*) indicated that e.g. it is not possible to control $A(\mathrm{o})$ by $C(\mathrm{o})$.

Let us suppose that a time record of an output cooling temperature $C(\mathrm{o})$ is available. Its qualitative interpretation is e.g.

$$C(\mathrm{o}) = (+,\, +,\, 0) \tag{75}$$

The qualitative interpretation of the quantitative additional information eliminates some qualitative states from the set of solutions (*74*).

$$\begin{array}{cccc} A(\mathrm{o}) & V(\mathrm{r}) & F(\mathrm{o}) & C(\mathrm{o}) \\ +,\,?,\,? & +,\,+,\,- & +,\,+,\,- & +,\,+,\,0 \end{array} \tag{76}$$

The result of the first level analysis is represented by (*74*) or (*77*) and Table IV. The second level is the system analysis.

Mixer-splitter analysis. The qualitative model of the mixer and the splitter is based on Eqs (*43*)–(*45*), (*47*), (*54*)–(*67*), (*69*). The following notation is used:

$$\begin{array}{llll} F(\mathrm{si}) = X(1) & A(\mathrm{i}) = X(6) & B(\mathrm{o}) = X(11) & T(\mathrm{so}) = X(16) \\ A(\mathrm{si}) = X(2) & B(\mathrm{i}) = X(7) & T(\mathrm{o}) = X(12) & F(\mathrm{re}) = X(17) \\ B(\mathrm{si}) = X(3) & T(\mathrm{i}) = X(8) & F(\mathrm{so}) = X(13) & A(\mathrm{re}) = X(18) \\ T(\mathrm{si}) = X(4) & F(\mathrm{o}) = X(9) & A(\mathrm{so}) = X(14) & B(\mathrm{re}) = X(19) \\ F(\mathrm{i}) = X(5) & A(\mathrm{o}) = X(10) & B(\mathrm{so}) = X(15) & T(\mathrm{re}) = X(20) \end{array} \tag{77}$$

The complete qualitative model is given in Table V. The explanation of blocks which are not given in (*28*) is presented as a set of remarks in Table V.

The variables $X(22)-X(37)$ are auxiliary variables and can be reconstructed from the complete qualitative model (see Table (V). As an example of the auxiliary variable the following is given

$$X(28) = X(5)^{*}\, X(8) \quad \text{see Eq. } (46)\,.$$

The first question is given in Table VI.

Q SENECA detects several inconsistencies. A simple inconsistency comes from the following

$$\begin{aligned} DX(1) &\leftarrow k0 \quad \text{see Table VI} \\ DX(17) &\leftarrow k+ \\ DX(5) &\leftarrow k- \,. \end{aligned} \tag{78}$$

TABLE V

Qualitative model of the mixer and splitter (see Fig. 1)

No.	Operation	Topology	No.	Operation	Topology
1	+	1, 17, 5	24	+	30, 35, 36
2	*	5, 6, 22	25	*	13, 16, 35
3	+	23, 24, 22	26	+	21, 37, 36
4	*	1, 2, 23	27	*	9, 12, 37
5	*	17, 18, 24	28	*M*54	2, 3, 0, see (*69*) for (si), see Fig. 1 $DA(\mathrm{si}) = -DB(\mathrm{si})$ 2, 3, 0
6	*	5, 7, 25	29	*M*58	$DDA(\mathrm{si}) = -DDB(\mathrm{si})$
7	+	26, 27, 25	30	*M*54	6, 7, 0
8	*	1, 3, 26	31	*M*58	6, 7, 0
9	*	17, 19, 27	32	*M*54	10, 11, 0
10	*	5, 8, 28	33	*M*58	10, 11, 0
11	+	29, 30, 28	34	*M*54	14, 15, 0
12	*	1, 4, 29	35	*M*58	14, 15, 0
13	*	17, 20, 30	36	*M*54	18, 19, 0
14	+	13, 17, 9	37	*M*58	18, 19, 0
15	*	9, 10, 31	38	*M*54	19, 17, 0
16	+	24, 32, 31	39	*M*45	18, 17, 0 see Eq. (*59*)
17	*	17, 18, 24	40	*M*45	9, 17, 0 see Eq. (*61*)
18	*	13, 14, 32	41	*M*49	9, 17, 0 see Eq. (*62*)
19	*	9, 11, 33	42	*M*45	12, 20, 0 see Eq. (*63*)
20	+	27, 34, 33	43	*M*12	37, 30, 0 see (*28*)
21	*	17, 19, 27	44	*M*12	30, 35, 0 see (*28*)
22	*	13, 15, 34	45	*M*12	13, 9, 0 see (*28*)
23	*	17, 20, 30	46	*M*13	13, 9, 0 see (*28*)

This first block (see Table V) gives

$$\begin{gathered} X(1) + X(17) = X(5) \\ \mathrm{D}X(1) + \mathrm{D}X(17) = \mathrm{D}X(5) \\ \mathrm{DD}X(1) + \mathrm{DD}X(17) = \mathrm{DD}X(5)\,. \end{gathered} \tag{79}$$

It is clear assignments (*79*), the Eq. (*80*), see (*6*)) are not consistent. Therefore a modification is needed.

The final result of man-machine dialogue through Q SENECA is given as the second question (see Table VI).

The model (see Table V) gives for the second question (see Table VI) 243 qualitative states provided that the set of interesting variables, see (*26*), is (see (*78*)):

$$1, 7, 10, 11, 13, 14, 15, 17, 18, 19, 20\,. \tag{80}$$

The first 27 solutions are described as follows

variable	X	DX	DDX	variable	X	DX	DDX
1	+	−	0	15	+	−	?
7	+	0	0	17	+	+	−
10	+	+	+	18	+	+	0
11	+	−	−	19	+	−	0
13	+	+	0	20	+	+	0
14	+	+	?	21	+	−	?

(*81*)

For simplicity let us suppose that the solution of mixer-splitter subsystem is represented by the matrix (*82*) only.

Coordination

The solution (*82*) of the mixer-splitter subsystem and the reactor solution (*74*) have the only "intersection". This intersection is variable $A(\mathrm{o})$, see $X(10)$ in (*82*) and $A(\mathrm{o})$ in (*74*)

	see (*82*)	see (*74*)
$A(\mathrm{o})$	+	+
$DA(\mathrm{o})$	+	?
$DDA(\mathrm{o})$	+	?

(*82*)

The matrix (*83*) represents the whole coordination. Its solution is very simple and is identical with the first column of the matrix (*83*).

Conclusion

A qualitative simulation of the chemical reactor is pre-processed. Some qualitative solutions are eliminated on the basis of the non qualitative analysis. Therefore the final qualitative description of the chemical reactor is not identical with its original qualitative model.
A model of the chemical reactor is a typical example of a transfer of conventional chemical engineering model into a qualitative model. A description of the splitter (Eqs (*54*)–(*67*)) is an example of a semisubjective model.

FERMENTATION

As a case study an anaerobic digestion is chosen. The original mathematical model is in ref.[14] and some qualitative features are given in ref.[21]. It is possible to increase gradually amount of knowledge. As suitable sources of additional knowledge the following was used[21–23]. However this modification is not presented here.

A set of qualitative relations based on the mathematical model[21,22] follows:

$$DX1 = -X2 - X1*X3 \tag{83}$$

$$X3 = X4 + X5 + X6 \tag{84}$$

$$X9 = X7/X8 \tag{85}$$

TABLE VI

Specification of the first version of the qualitative question for the model given in Table V, the second question is a result of man machine dialogue

Variable	1st Question			2nd Question			Variable	1st Question			2nd Question		
	X	DX	DDX	X	DX	DDX		X	DX	DDX	X	DX	DDX
1	+	0	0	+	?	0	11	+	+	+	+	?	?
2	+	0	0	+	0	0	12	+	+	+	+	+	+
3	+	0	0	+	0	0	13	+	+	0	+	?	0
4	+	0	0	+	0	0	14	+	?	?	+	?	?
5	+	–	–	+	–	–	15	+	?	?	+	?	?
6	+	0	0	+	0	0	16	+	0	0	+	0	0
7	+	+	?	+	?	?	17	+	+	+	+	?	?
8	+	+	–	+	+	–	18	+	+	?	+	?	?
9	+	+	–	+	+	–	19	+	0	0	+	?	0
10	+	+	–	+	?	?	20	+	0	0	+	?	0
							21–37	?	?	?	?	?	?

$$X8 = X10 - X11 \tag{86}$$

$$DX10 = X12*(X13 - X10) \tag{87}$$

$$X2 = X14 - X7 \tag{88}$$

$$X14 = X1 \tag{89}$$

$$DX15 = X12*(X16 - X15) \tag{90}$$

$$DX7 = X12*(X17 - X7) \tag{91}$$

$$X19 = X12*(X20 - X8) + DX11 - DX10 \tag{92}$$

$$DX22 = X12*(X21 - X22) + X23*X22 - X15 \tag{93}$$

$$DX11 = X12*(X24 - X11) - X23*X22 \tag{94}$$

$$X23 = m/(1 + Ks/X25 + X25/K1) \tag{95}$$

$$X18 - X22*X23 \tag{96}$$

$$X5 = X22*X23 \tag{97}$$

$$X4 = -X2 \tag{98}$$

$$X25 = X11*X9 \tag{99}$$

where

X_1 is pCO_2 – partial pressure of carbon dioxide, $X2$ is TG – rate of gas transfer, $X3$ is Q – total off-gas flow, $X4$ is QCO_2 – carbon dioxide flow rate into gas phase, $X5$ is QCH_4 – methane rate of production, $X6$ is QH_2O – rate of water vapour entering or leaving the gas phase, $X7$ is $(CO_2)D$ – concentration of dissolved carbon dioxide, $X8$ is (HCO_3^-) – concentration of bicarbonate ion, $X9$ is (H^+) – hydrated hydrogen ion concentration, $X10$ is z – net cation concentration, $X11$ is s – substrate concentration, $X12$ is F – hydraulic flow rate, $X13$ is zo – z (see $X10$) in the input stream, $X14$ is $(CO_2)D^*$ – saturated concentration of carbon dioxide in solution, $X15$ is tox – concentration of toxic chemical agent, $X16$ is toxo – tox (see $X15$) in the input stream, $X17$ is $(CO_2)Do$ – (CO_2) see ($X7$) in the iput stream, $X18$ is RB – rate of biological production of carbon dioxide, $X19$ is R – net rate of chemical production of dissolved carbon dioxide, $X20$ is $(HCO_3^-)_0$ – (HCO_3^-) (see $X8$) in the input stream, $X21$ is xo – x (see $X22$) in the input stream, $X22$ is x – biomass concentration, $X23$ is m – specific growth rate, $X24$ is so – s (see $X11$) in the input stream, $X25$ is (hs) – ionized substrate concentration, $X26$ is VFA – volatile fatty acid, $X27$ is VFAo – VFA (see $X26$) in the input stream, are qualitative variables.

The following constants (see refs[21,22]):
p, V, VG, mmax, $K1$, kLa, k, Yx/s, YCO_2/x, YCH_4/x, Ka are positive and multiplicative. Therefore they are ignored in the Eqs (*84*)–(*95*), (*97*)–(*100*). The constants mmax, K, $K1$ are positive (see Eq. (*96*)) and additive.
The original mathematical model (see refs[21,22]) does not include volatile fatty acid (VFA = $X26$). Therefore the equation oriented qualitative model (*84*)–(*100*) cannot answer any qualittive question connected with VFA.
A non-equation based (i.e. shallow qualittive) knowledge is available concerning mutual relationships among VFA and some others variables using parametric derivatives (see Table VII and (*28*)).

Input variable	No. of block type (see Table VII)	Output variable	
VFA ($X26$)	$M24$	(HCO_3^-) ($X8$)	(*100*)
VFAo ($X27$)	$M25$	(HCO_3) ($X8$)	
VFAo ($X27$)	$M22$	(toxo) ($X16$)	(*102*)
VFAo ($X27$)	$M24$	$(HCO_3^-)_0$ ($X20$)	(*103*)
VFA ($X26$)	$M22$	(tox) ($X15$)	(*104*)
F*so*x ($X60$)	$M34$	(pCO_2) ($X1$)	(*105*)

The Eq. (*94*) can be for the positive values of m and (hs) described by the following M block (see (*28*) and Table VIII):

$$(hs)\quad (X25)\quad M29\quad m(X23)\,. \tag{106}$$

TABLE VII
Specification of parametric derivatives see (*10*), (*11*), (*28*))

Identification symbol	DX_j/DX_i	DDX_j/DDX_i	Identification symbol	D/D	DD/DD	Identification symbol	D/D	DD/DD	X_i	X_j
$M21$	+	+	$M22$	+	0	$M23$	+	–	$k0$	$k+$
$M24$	–	+	$M25$	–	0	$M26$	–	–	$k0$	$k+$
$M27$	+	+	$M28$	+	0	$M29$	+	–	$k0$	$k0$
$M30$	–	+	$M31$	–	0	$M32$	–	–	$k0$	$k0$
$M33$	+	+	$M34$	+	0	$M35$	+	–	$k0$	$k-$
$M36$	–	+	$M37$	–	0	$M38$	–	–	$k0$	$k-$

The Eq. (*99*) is the block

$$X4 \quad M4 \quad X2\,. \tag{107}$$

Let a control system be represented by three control loops:

controller input	No. of M block (see Table VII)	controller output	
$so(X24)$	$M29$	$QCH_4\,(X5)$	(*108*)
$so(X24)$	$M34$	$s\quad(X11)$	(*109*)
$F^*so(X57 = X24^*X12)$	$M29$	$x\quad(X22)$	(*110*)

variable so is the key control variable. It effects, through the controller loops (*109*), (*110*), (*111*), other variables. This fact makes the qualitative model much more interconnected.

A bioengineer must keep in mind that a commonsense engineering background is not available to a computer. In this specific case a naive physical chemistry is needed. However it is not available.

TABLE VIII

Specification of blocks which are based on qualitative parametric derivative

Blocks	Eq.	Blocks	Eq.
$X28 = DX1$	*84*	$X44 = X12^*X17$	*92*
$X29 = X2 + X28$	*84*	$X45 = X19 + X33$	*93*
$X30 = X1 + X3$	*84*	$X46 = X8^*X12$	*93*
$X32 = X4 + X6$	*85*	$X47 = X12^*X20$	*93*
$X33 = DX10$	*88*	$X48 = DX11$	*93*
$X34 = X10^*X12$	*88*	$X49 = X47 + X48; X46 + X45$	*93*
$X35 = X12^*X13; X33 + X34$	*88*	$X50 = DX22$	*94*
$X36 = DX15$	*91*	$X51 = X12^*X22$	*94*
$X37 = X12^*X15$	*91*	$X52 = X12^*X21$	*94*
$X38 = X36 + X37; X12^*X16$	*91*	$X53 = X22^*X23$	*94*
$X39 = DX7$	*92*	$X54 = X52 + X53; X15 + X55$	*94*
$X40 = X7^*X12$	*92*	$X55 = X50 + X51$	*94*
$X41 = X39 + X40; X19 + X42$	*92*	$X56 = X11^*X12$	*95*
$X42 = X18 + X43$	*92*	$X57 = X12^*X24; X58 + X53$	*95*
$X43 = X2 + X44$	*92*	$X58 = X48 + X56$	*95*

The following inequalities represent the commonsense engineering background in the qualitative model of the anaerobic digestion

$$X11 < X24 \quad s < so \tag{111}$$

$$X22 > X21 \quad x > xo \tag{112}$$

$$X15 < X16 \quad \mathrm{tox} < \mathrm{toxo} \tag{113}$$

$$X17 > X7 \quad (\mathrm{CO_2})\,\mathrm{Do} > (\mathrm{CO_2})\,\mathrm{D} \tag{114}$$

$$X14 > X7 \quad (\mathrm{CO_2})\,\mathrm{D}^* > (\mathrm{CO_2})\,. \tag{115}$$

An engineering experience is described by the following three inequalities

$$X5 > X18 \quad Q\mathrm{CH_4} > Q\mathrm{CO_2} \tag{116}$$

$$X4 > X6 \quad Q\mathrm{CO_2} > Q_2\mathrm{O} \tag{117}$$

$$X5 > X18 \quad Q\mathrm{CH_4} > \mathrm{RB}\,. \tag{118}$$

The inequalities (*117*), (*118*), (*119*) can be broken under certain conditions. They are not based on laws of nature.

A specification of a problem for Q SENECA requires an introduction of auxiliary variables (see Table VIII). The last column of Table VII indicates a number of the equations (see (*49*)–(*79*)). E.g. the first line of the Table VIII gives

$$X28 = \mathrm{D}X1\,.$$

In Table IX there is a partial specification of the qualitative mode (the first 10 blocks out of a set of 64 blocks which represents the complete model). The last column of this table indicates a number of equations (*84*)–(*119*). An example of a qualitative question is given in Table X.

A bad digestion operation is specified qualitatively as follows (experts opinion):

		X	DX	DDX
$p\mathrm{CO_2}$	$X1$	+	+	+
T	$X2$	+	−	−
$Q\mathrm{CH_4}$	$X5$	+	−	−
$(\mathrm{HCO_3^-})$	$X8$	+	−	−
tox	$X15$	+	+	+

(*119*)

Let us suppose that the main goal of the qualitative study is to make a list of all qualitative states under which the bad digestion (*120*) can occur. In this case the assignments (*120*) represent a subquestion.
The question in Table X is transferred into a general question Q if it gives only general deep knowledge. In the specific case of the Table X the general question is

TABLE IX
Qualitative model the anaerobic fermentor

Block No.	Type	Topology	Eq.
1	$M5$	1, 28, 0	*84*
2	$M6$	2, 28, 29	*84*
3	$M4$	29, 30, 0	*84*
4	$M7$	1, 3, 30	*84*
5	$M6$	4, 6, 32	*85*
6	$M6$	5, 32, 3	*85*
7	$M7$	8, 9, 7	*86*
8	$M6$	8, 11, 10	*87*
9	$M5$	10, 33, 0	*88*
10	$M7$	10, 12, 34	*88*

TABLE X
Qualitative question answered by the fermentor qualitative model (see Table IX)

Variable	X	DX	DDX	Variable	X	DX	DDX
$X1$	+	−	−	$X15$	+	+	+
$X2$	+	−	−	$X16$	+	+	?
$X3$	+	+	?	$X17$	+	?	?
$X4$	+	−	−	$X18$	+	?	?
$X5$	+	?	?	$X19$	+	0	0
$X6$	+	?	?	$X20$	+	?	?
$X7$	+	?	?	$X21$	+	−	−
$X8$	+	−	?	$X22$	+	+	?
$X9$	+	?	?	$X23$	+	?	?
$X10$	+	?	?	$X24$	+	−	−
$X11$	+	?	?	$X25$	+	?	?
$X12$	+	0	0	$X26$	+	?	?
$X13$	+	0	0	$X27$	+	+	+
$X14$	+	+	+				

$$X(i) = + \; ; \quad DX(i) = ? \; ; \quad DDX(i) = ? \quad i = 1, 2, \ldots, 27 \, . \qquad (120)$$

Both questions (the first question is represented by Table X, the second one specific by (*121*)) were submitted for analysis by the model in Table IX. Both questions cannot be answered because of the model and the questions inconstancies.

Q SENECA indicates all inconsistencies. A transparency of the reasoning mechanism is guaranteed through the expert system itself. From Eqs (*89*) and (*116*) the following results are obtained:

$$X2 = k+ \, . \qquad (121)$$

The value of $X4$ (see Table X or (*121*)) is

$$X4 = k+ \, .$$

However the Eq. (*99*) requires either

$$X2 = k- \qquad (122)$$

or

$$X4 = k- \, . \qquad (123)$$

However Table X and Eq. (*121*) give positive values for both variables.

Let us suppose that an expert after a commonsense analysis of an interaction of anaerobic microorganisms and CO_2 concentration accepts

$$X4 = k- \, . \qquad (124)$$

The new question Q, which corresponds to the above given modification, differs from Table X only in the 4th row

variable	X	DX	DDX
$X4$	?	?	?

Another alternative is to change the equation (*99*) into

$$X4 = X2 \qquad (126)$$

and keep Table X unchanged.

For the brevity sake the model partially given by Table IX with the following modification

$$3 \quad M3 \quad 29 \quad 30 \quad 0 \qquad (127)$$

is studied.

Qualitative Projection

The following three groups of interesting variables $I1$, $I2$, $I3$ (see (*26*)) are studied:

Group 1, list of $I1$: (*128*)

Q, QH_2O, (CO_2) D, (HCO_3^-), (H^+), z, s, $(HCO_3^-)_0$, m, (hs), VFA, it means $X5$, $X6$, $X7$, $X8$, $X9$, $X10$, $X11$, $X20$, $X23$, $X25$, $X26$.

Group 2, list of $I2$: (*129*)

QCH_4, F, xo, VFA, it means $X5$, $X12$, $X21$, $X26$.

Group 3, list of $I3$: (*130*)

F, xo, x, so, it means $X12$, $X21$, $X22$, $X24$.

Every group represents a certain "qualitative projection" (point of view) of thə same anaerobic qualitative model (see Table IV, (*128*)). An engineering interpretations of these points of views are:

Group 1 (see (*129*)): set of such variables that are not specified by the question in Table X

Group 2 (see (*130*)): methane production

Group 3 (see (*131*)): organic overloading

Some variables given in (*129*), (*130*), (*131*) are fully or partially specified by Table X, namely

Group 1 $X8 = (+, -, ?)$

Group 2 $X12 = (+, 0), X21 = (+, -, -)$ (*131*)

Group 3 $X12 = (+, 0, 0), X21 = (+, -, -), X2 = (+, +. ?)$

A comparison of (*129*) and (*132*), (*130*) and (*132*), (*131*) and (*132*) gives these variables which are interesting (see (*26*)) and are not specified by the question (see Table X). Answers of the question (see Table X) using interesting and previously not specified variables are:

Group 1 (see (*129*)): there a more than 400 solutions. Therefore the secondary projection is needed to decrease a number of variables. Some of the solutions in 5 dimensional qualitative space are:

qualitative state No.	$X6$	$X9$	$X20$	$X23$	$X25$
1	+, +, +	+, +, +	+, −, +	+, +, +	+, +, +
64	+, +, 0	+, +, 0	+, −, +	+, +, −	+, +, 0
67	+, +, 0	+, +, 0	+, −, 0	+, +, 0	+, +, +
69	+, +, 0	+, +, 0	+, −, 0	+, +, −	+, +, 0
130	+, +, −	+, +, −	+, −, 0	+, +, −	+, +, −
150	+, 0, −	+, +, −	+, −, −	+, +, −	+, +, −

(*132*)

The variables not given in (*133*) are identical in all qualitative states with these qualitative values given in Table X

Group 2

$X5$	$X12$	$X21$	$X26$
+, +, −	+, 0, 0 (see (*132*)	+, −, − see (*132*)	+, +, +

(*133*)

Group 3

state No.	$X12$	$X21$	$X22$	$X24$
1	+, 0, 0	+, −, −	+, +, +	+, +, −
2	+, 0, 0	+, −, −	+, +, 0	+, +, −
3	+, 0, 0	+, −, −	+, +, −	+, +, −

(*134*)

The only difference among states Nos 1, 2 and 3 is the sign of the third derivative of $X22$. Therefore the following condensed specification of the (*135*)

1, 2, 3 +, 0, 0 +, −, − +, +, ? +, +, − .

The set of qualitative states is not the final result of a qualitative simulation. Very important for any bioengineering qualitative study is the knowledge of possible transition among all qualitative states i.e. state diagram. A simplified list of all possible transitions is given in Table XI. Only two types of transitons are considered, namely A and B. For details see refs[16,17].

The first row of Table XI indicates that there is only one possible transition from the triplet (+ + +). This transition is a transition of type A and the resulting qualitative state is described by the triplet (+ + 0).

The following qualitative transitions cannot be rejected because of the unknown third derivative

No.		from state		to state			
	X	DX	DDX	DDDX	X	DX	DDX
1	?	?	+	+	?	?	+
2	?	?	+	0	?	?	+
3	?	?	+	−	?	?	0
4	?	?	0	+	?	?	+
5	?	?	0	0	?	?	0
6	?	?	0	−	?	?	−
7	?	?	−	+	?	?	0
8	?	?	−	0	?	?	−
9	?	?	−	−	?	?	−

where ? means any qualitative value. The transition of this nature are transition of type A (see Table XI).
Transition B can be explained through a definition of a derivative itself. If there are different qualitative values of the first and the second derivatives (variable value and the first derivative) then the first derivative (the value of variable) will be changed in a proper way.
Some transitions among the states (*133*) are given in (*137*). The following general form of specification is given

TABLE XI
A partial list of commonsense transitions among 27 one dimensional qualitative states

No.	Transitions	No.	Transitions
1	+++A++0	15	00−
2	++0A+++A++	16	0−+B−−+
3	++−A++0 B+0−	17	0−0 B−−+ B−−−
4	+0+ B+++	18	0−− B−−−
5	+00	19	−++ A−+0 B0++ B0+0
6	+0− B+−−	20	−+0 A−++ A−+− B0+0
7	+−+ A+−0 B+0+ B0−+ B0−0	21	−+− A−+0 B−0− B0+0
8	+−0 A+−+ A+−− B0−0	22	−0+ B−++
9	+−− A+−0 B0−− B0−0	23	−00
10	0++ B++0 B++− B+++	24	−0− B−−−
11	0+0 B++0 B++0 B+++	25	−−+ A−−0 B−0+
12	0+− B++−	26	−−0 A−−+ A−−−
13	00+ B+++	27	−−− A−−0
14	000		

transition No. from qualitative state *(135)*
transition type (see Table XI)
to qualitative state

The following transition matrix gives all possible transitions among states (*133*)

	from to	$X6$ $X6$	$X9$ $X9$	$X20$ $X20$	$X23$ $X23$	$X25$ $X25$
1	1	$++ +$	$+++$	$+-+$	$+++$	$+++$
		A	A	A	A	see Table XI
	67	$++0$	$++0$	$+-0$	$++0$	$+++$
2	64	$++0$	$++0$	$+-+$	$++-$	$++0$
				A	A	A
	67	$++0$	$++0$	$+-0$	$++0$	$+++$
3	64	$++0$	$++0$	$+-+$	$++-$	$++0$
				A	A	A
	69	$++0$	$++0$	$+-0$	$++-$	$++0$
4	64	$++0$	$++0$	$+-+$	$++-$	$++0$
		A	A	A		A
	130	$++-$	$++-$	$+-0$	$++-$	$++-$
5	69	$++0$	$++0$	$+-0$	$++-$	$++0$
		A	A			A
	130	$++-$	$++-$	$+-0$	$++-$	$++-$
6	130	$++-$	$++-$	$+-0$	$++-$	$++-$
		B		A		
	150	$+0-$	$++-$	$+--$	$++-$	$++-$

(136)

The transition No. 1 from the state No. 67 (see (*133*) is caused by A transition (see (*11*)) of variables $X6, X9, X20$ and $X23$ (see (*133*) and (*137*)). Variable $X25$ is constant i.e. its qualitative triplet (see (*4*)) is identical in the states 1 and 67. The transition of variable $X6$ of the first transition (see (*137*), the first row) is described by the first row of Table I (therefore $A(1)$ in (*137*)). It is clear e.g. that the state No. 67 is a terminal.

There is the only qualitative solution (see (*134*)) for the second group of variables (*130*). The variable $X5$ (QCH_4) goes up, however it will reach a certain maximum (i.e. $DX5 = k0$). The variable $X26$ (VFA) goes up more and more quickly ($DX26 = k+$, $DDX26 = k+$).
A natural complexity of an extremely sophisticated systems as microorganism (indirectly fermentors) can only be described by a model consisting of many relatively simple projections (point of views). Each of these views captures one level of details, linked by abstraction of different relations (probably using different calculi). This is perhaps an "intelligent approach" for biotechnological tasks. Integration of different types of bioengineering knowledge (e.g. fuzzy, rough, cognitive qualitative) is the next logical step toward an expert system of the second generation.

CONCLUSION

Less information intensive i.e. usually less accurate model of a large system can be more realistic. It can reflect reality in its complexity. A numerical model is always simplified and highly specialized. Therefore qualitative models are very useful provided complex and ill known processes are studied.
Perhaps the most frequent area of application of qualitative modelling is a diagnosis. See e.g. ref.[1]. This is an indirect evidence that qualitative modelling can solve industrial tasks. Diagnosis of large system requires decomposition.
Many bottlenecks are known that constrain areas of qualitative model applicability e.g.: integration of shallow and deep knowledge; elimination of quantitatively non existing (spurious) solutions (state); development of more efficient qualitative algorithms; minimization of computer (memory time).
The decomposition of large models and consequently coordination of subproblems must be solved provided industrial problems are studied. Very often a system is decomposed into a control system and a process itself. Safety (loss prevention) specifications are presented in this way.
Case studies given in this paper are rather simple. However they are not purely academic problem (especially the fermentor model).
Perhaps a qualitative model is not general enough to cover requirements of practical applications. Therefore even more general approach will be needed. A semiqualitative model seems to be a natural candidate[24].

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