NAIVE MODELS AS ACTIVE EXPERT SYSTEM IN BIOENGINEERING AND CHEMICAL ENGINEERING

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A possibility of qualitative variable utilization for description and evaluation of phenomena and processes from non-formal human thinking point of view is presented. Paper gives methods of naive modelling and realistically assesses results that can be awaited. The method is demonstrated on two case studies that are given in full details, namely continuous fermentation (fermentor, two separators) and anaerobic fermentation.

Expert systems have been employed in some branches (e.g. medicine, geology) for 15 years[1]. Recently expert systems have been utilized in process industry (see e.g. refs[2-5]). Their using is very variable. On the basis of information from knowledge base an answer to a question is searched (see e.g. ref.[2]). Expert systems are also used as intelligent regulators[6] or they can be utilized as a part of a more complex model[7] that is not composed of an expert system or a network of expert systems[8]only.

Current expert systems of the first generation are able to search through an expert base by a relatively nonflexible, i.e. in advance less or more fixed way. Their main disadvantage, in comparison to a human being is that they are not capable of "human" reasoning[9] (common sense).

On the other hand the expert systems of the first generation are not recommended for such problems that need a common sence reasoning. The problem is, that just these points are important in practice. A diagnostics problem can be given as an example.

If diagnostics is approached as it is common at expert systems using, no too good results are achieved. Procedure does not rest upon elaboration of lists of symptoms and failures and following co-ordination of symptoms to failures only. Basic reasons why exploitation of pattern recognition (see e.g. ref.[10]) is not succesfull are following:

- measurements are very inaccurate, especially at biotechnologies where distinctive variation of live material exists;
- it is impossible to work out a complete list of failures and their symptoms;
- failures can be structured;
- slow and therefore with difficulty detected trends appear.

An expereinced, careful and sufficiently patient expert/team of experts is/are able to detect failures much better than an expert system without commonsence reasoning[11].

Similar conclusions are drawn in a number of other subjects of study, for example:

- identification of molecule form[12] (reaction scheme)
- chemical technology synthesis[13]
- operative control of multipurpose and multiproduct production[14]
- microorganism behaviour[15]
- influence of genetics on biotechnology behaviour[16].

There are many problems that influence technical level of biochemical and chemical equipment closely, beyond the region of process engineering, for instance:

- properties of metal and non-metal materials[17,18]
- corrosion protection
- creeping properties
- in combination with mechanical stress
- vibration diagnostics[19]
- automation of failures tree creation (causal trees)[20].

The situation is complicated by the fact that there is a lack of expert engineers and highly qualified experts who would be able to create necessary expert basis.

For a long time practice has made a pressure on development of new methods that would be capable of semicreative work on a level comparable to human being. That was the reason why naive physics has come into being[21,22]. This non-numerical physics is purely, or almost purely causal.

It is understandable that algorithms worked out on the naive physics principle are not better then an experienced expert. In comparison to previous generation of expert systems the "naive" expert systems are much more "powerful". There are also a few algorithms that start from the base philosophy of naive physics. See e.g. refs[23-25].

Following simple problem demonstrates clearly causal binding. In an intensimaly small vessel flux 1, rate of flow Q_1 (kg s^{-1}) flows. Fluxes number 2 and 3, rates of flows Q_2 and Q_3 flow out of that vessel. Balance equation for this point is

$$Q_1 = Q_2 + Q_3 \, .$$

It is, for instance, obvious that under constant flux Q_2 relation

$$Q_3 = f(Q_1)$$

is pure monotonic. Algorithmes published in papers[23-25] are based on similar reasonings and their algorithmization.

A confluence method has been chosen for its direct applicability[24].

Confluence

Roughly speaking, confluence is an equation in which qualitative derivations (quantities) occur. Qualitative derivations (quantities) are such derivations that aquire discrete sets of values only. Further exclusively three-value qualitative derivations (falling = −, growing = +, constant = 0) will be used. Five-value qualitative derivation has been used in paper[22].

Manipulation of qualitative derivations (quantities) is based on elementary knowledge of arithmetics. For multiplication and addition operations the knowledge is summarized into two matrices (*1*) and (*2*).

$$\begin{array}{cc|ccc} & & & x_2 & \\ & & + & 0 & - \\ \hline x_1 & + & + & + & x \\ & 0 & + & 0 & - \\ & - & x & - & - \end{array} \qquad x_1 + x_2 \qquad (1)$$

$$\begin{array}{cc|ccc} & & & x_2 & \\ & & + & 0 & - \\ \hline x_1 & + & + & 0 & - \\ & 0 & 0 & 0 & 0 \\ & - & - & 0 & + \end{array} \qquad x_1 \,.\, x_2 \qquad (2)$$

Symbol x is used for result designation that can have any qualitative value, i.e. + or − or 0. Existence of such a result is obvious. If absolute values X_1 and X_2 are not known it is impossible e.g. to predict the sign of their difference $X_1 - X_2$.

Linear confluence has the form

$$R_i = \sum_{i=1}^{n} K_i X_i \,, \qquad (3)$$

where R_i and K_i are qualitative values, hence values +, − or 0. Quantities X_1 are qualitative derivations (quantities). Any other confluences are non-linear ones.

The simplest algorithm for solution of confluence system is probably a "rough force". Suppose we have n qualitative quantities, then it is possible to generate all potential qualitative solutions without problems. Then there are 3^n of total potentional solutions since three qualitative values are considered.

Each of this potentional solution is verified towards all confluences in the set of confluences. The potentional solution corresponding all confluences is then solution of confluence system.

For large systems of confluences this procedure is less convenient[26]. Advantage of it is obvious because any confluence systems can be solved, even non-linear. In paper[27] an effective algorithm of linear confluence system is shown. Since qualitative linearization is relatively simple, it is possible, by repeating of solution of linear confluence system, to solve even a system of non-linear confluences.

Mathematical aspects of solution of confluence system are not obvious so far. A specialized algebra have to be worked out, probably. Especially difficult may be a creation of a qualitative analogy to numerical mathematics. It may take a long time. But even by means of simple algorithms for solution of linear confluence systems it is possible to solve a number of interesting problems. However mathematical point of view is not purpose of this paper.

One of the most important, may be the basic reason, why qualitative model is important so much for biotechnologies and for chemical industry, lies with the fact that it is a probably complete generator of all possible alternatives. This feature is extraordinary important especially where problems of reliability are in question. In these cases specially one must be sure that no hazardous situation has been ommited.

Causal Graphs

Set of qualitative solutions is an interresult only in the course of application of qualitative models. This result should be arranged appropriately, to be simple and suitable for answer searching from human point of view. Engineering interpretation of qualitative solution is in fact a qualitative description of behaviour of the studied system. To be able to utilize a set of qualitative solutions a proper structure is necessary to introduce into set of solutions. Otherwise the set of qualitative solutions is not well-arranged.

Especially negative is a case where number of qualitative solutions is several hundreds or thousands. Number of solutions of a relatively simple problem (see ref.[28]) has exceed one thousand.

It turned out that it is suitable to determine a primary set of qualitative values and then a sequence of causal tree branching .Let us have set of all qualitative variables

$$X \equiv \{X_1, X_2, \ldots, X_n\} \,. \tag{4}$$

Primary set of qualitative values is a set of qualitative values a (see (*6*)) certain subset of qualitative quantities X_{P}

$$X_{\mathrm{P}} \equiv \{X_{\mathrm{P}_1}, X_{\mathrm{P}_2}, \ldots, X_{\mathrm{P}_s}\} \subset X \tag{5}$$

$$X_{\mathrm{P}_1} = a_{\mathrm{P}_1}$$

$$\begin{array}{c} X_{P_2} = a_{P_2} \\ \vdots \quad\;\; \vdots \\ X_{P_s} = a_{P_s} \\ a \equiv \{a_{P_1}, a_{P_2}, \ldots, a_{P_s}\} \,, \end{array} \qquad (6)$$

where s is cardinality of set P. P is a subset of indexes

$$P \subset \{1, 2, \ldots, n\} \,. \qquad (7)$$

From engineering point of view a set of primary qualitative quantities (5) is such a set of quantities, by means of that it is possible qualitatively describe state (6), in which system under study is. All qualitative quantities that are not involved in primary set

$$X_{C_1}, X_{C_2}, \ldots, X_{C_{n-s}} \qquad (8)$$

are considered to be causal qualitative quantities. Set of indexes of these quantities is

$$C \equiv \{1, 2, \ldots, n\} - P \,. \qquad (9)$$

An user of qualitative model may determine any succesion of branching of causal qualitative variable subset. Indexes of this subset forms set K

$$K \subset C \qquad (10)$$

cardinality of set K is k.

If a set of primary qualitative quantities (5) is selected, a causal tree may be generated, which branching is given by sequence

$$X_{K_1}, X_{K_2}, X_{K_3}, \ldots, X_{K_k} \qquad (11)$$

as it is shown in Fig. 1, where S_{X_k} is a set S of qualitative solutions which corresponds to the branching sequence (11). This figure shows that for beforehand given values of primary qualitative quantities (PMQV) the quantity X_{K_1} is branched as the first. Branching proceeds as long as all quantities of the sequence (11) are branched. Every possible path from PMQV to node X_{K_i} for $1 \leqq j \leqq k$ a set of qualitative solutions, corresponding to this path may be determined. Only one from all possible subsets of qualitative solution is shown in Fig. 1. The set of qualitative solutions corresponds to such a path that is characterized by qualitative values equal to zero for all causal variables (11).

Under certain circumstances the causal tree shown in Fig. 1 may be considered to be "anti-causal". The anticausal tree determines what kind of qualitative values (*11*) must be, to reach qualitative values (*6*) of primary set (*5*).

Problems of Testing

Since the point at issue is new in biotechnology and chemical engineering, two distinctive different problems were selected as test ones. The first problem has a system character. Qualitative models of individual nodes are very simple.

The second model is based on a real model of anaerobic ferementor. Thus only one apparatus is represented by model. It has not originated on the basis of speculation as the previous model has – but on basis of conventional model. Technological scheme of fictive continual biotechnology is shown in Fig. 2. Node *1* is a homogenization tank. Node *2* is a continual mixed fermentor. Node *3* is a centrifuge, where biomass B is separated from product P and substrate S. If flow of biomass in flux *3* is bigger than a certain threshold flowrate *V* then quantity of biomass being in excess of mentioned minimum flowrate *V* passes into flux *4*. Neither product nor substrate flow in branch *7*.

Node *4* is distillation, it separates product and substrate. Separation is not perfect and both product and substrate are in fluxes *5* and *6*. Biomass that gets into flux *4* leaves system in flux *5*. Complete qualitative model has already been published[28].

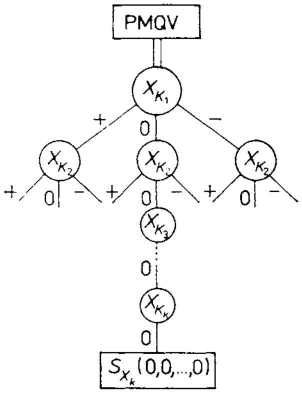

FIG. 1

Causal tree with given set of primary qualitative values (PMQV)

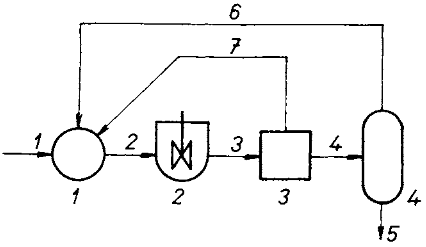

FIG. 2

Flow sheet of continuous biotechnology. Node *1* mixer, node *2* fermentor, node *3* separator of biomass, node *4* separator of substrate and product

Since algorithm used for solution of confluence system is defined for solution of linear confluence only, non-linear relations must be linearized. Validity of the linearized confluences is limited and therefore several systems of confluences must be considered.

One non-linearity has already been discussed briefly. It has been caused by limited capacity of quantity V of centrifuge (node 3). Qualitative graph characterizing centrifuge behaviour is shown in Fig. 3. Owing to qualitative model of centrifuge two systems of confluences, for flow of biomass in the third flux B_3, must be considered. If

$$B_3 \leqq V \tag{12}$$

centrifuge is in state s_1 (see Fig. 3). If

$$B_3 > V \tag{13}$$

centrifuge is in state s_2.

Qualitative characterization of fermentor is more complicated and it needs definition of more states. In Figs 4 and 5 are shown non-linear dependences that have been considered. It is biomass production in fermentor B_F as function of temperature in fermentor T (see Fig. 4) and dependence of biomass production in fermentor B_F as function of product flux P_3 (product concentration) in the third stream (see Fig. 5). Biomass production in fermentor B_F is qualitative function of two independent variables. We suppose that form of the function follows from intersection of function shown in Figs 4 and 5. Plan view of this intersection, under pressumption that (see Figs 4 and 5)

$$TO = UO$$

is shown in Fig. 6.

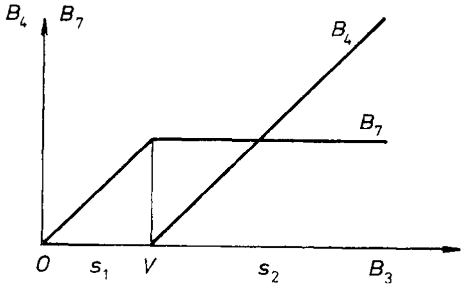

FIG. 3

Graphical record of qualitative behaviour of biomass separator (node 3 in Fig. 2) in states s_1 and s_2

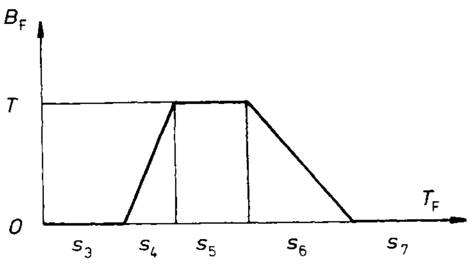

FIG. 4

Qualitative description of dependence of biomass production B_F vs fermentation temperature T_F for states s_3—s_7

System of confluences taken from literature[28] does not describe all combinations of states. It is because of demonstration of possibility to work with incomplete qualitative model. However sometimes a very rapid increase of qualitative solutions occurs.

To distinguish qualitative values +, −, 0 unambigously from their original meanings, symbols $k+$, $k-$, $k0$ will be used for them, hereafter. Hence confluence

$$X_1 = k+ \tag{14}$$

means that qualitative quantity X_1 is positive.

Confluences considered in test example are taken from literature[28] (subscribes specify number of stream – see Fig. 2, subscribe F is fermentor):
The set of confluences is formed by two subsets namely by a bilance subset and a model subset. The bilance subset indicates which qualitative variable is considered as constant or equal to zero.
bilance subset

mixer node *1*, Fig. 2

$$DS_1 + DS_6 = DS_2$$
$$DP_6 = DP_2$$
$$DB_7 = DB_2$$

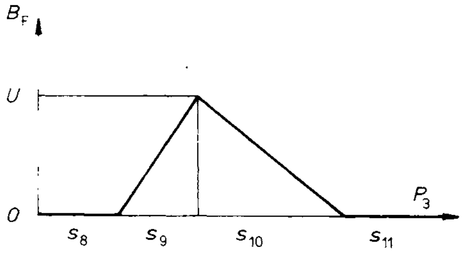

FIG. 5

Qualitative description of dependence of biomass production B_F vs product concentration, characterized by flow of product in the third flux P_3 (see Fig. 2)

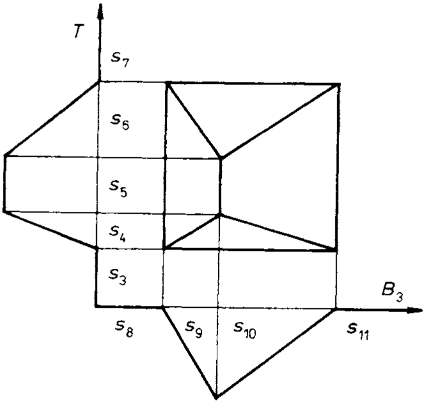

FIG. 6

Two-dimensional qualitative description of fermentor (node *3* in Fig. 2) formed on basis of one-dimensional descriptions from Figs 4 and 5 fermentor node *2*, Fig. 2

$$\begin{aligned} DP_3 &= DP_2 + DP_F \\ DB_3 &= DB_2 + DB_F \\ DS_2 &= DS_3 + DS_F \end{aligned} \tag{15}$$

separator node *3*, Fig. 2

$$\begin{aligned} DS_3 &= DS_4 \\ DP_3 &= DP_4 \\ DB_2 &= DB_4 + DB_7 \end{aligned}$$

distillation node *4*, Fig. 2

$$\begin{aligned} DB_4 &= DB_5 \\ DP_4 &= DP_5 + DP_6 \\ DS_4 &= DS_5 + DS_6 \end{aligned}$$

model subset

mixer
no model confluence
fermentor

$$\begin{aligned} DS_F &= DB_F + DP_F \\ DB_F &= (k_T \,.\, DT_F + k_P \,.\, DP_3)\, k \,, \end{aligned}$$

where (see Fig. 4)

k_T	$k0$	$k+$	$k0$	$k-$	$k0$
state s	s_3	s_4	s_5	s_6	s_7

and (see Fig. 5)

state s	s_8	s_9	s_{10}	s_{11}
k_{P_3}	$k0$	$k+$	$k-$	$k0$

The qualitative constant k is always

$$k = k+$$

with the following exception
if $k_T = k0$ or $k_B\mathrm{f} = k0$ then $k = k0$

separator

$$\begin{aligned} DB_7 &= k_B\mathrm{f} \,.\, DB_3 \\ DB_4 &= k_B\mathrm{f} \,.\, DB_3 \,, \end{aligned}$$

where see Fig. 3

state	s_1	s_2
$k_B\mathrm{f}$	$k0$	$k+$
$k_B\mathrm{f}$	$k+$	$k0$

distillation

$$\begin{aligned} DS_6 &= DS_4 \\ DS_5 &= DS_4 \\ DP_6 &= DP_4 \\ DP_5 &= DP_4. \end{aligned}$$

Original set of confluences (*15*) may be simplified with help of substitutions:

$$\begin{aligned} X_1 &= DS_1 \\ X_2 &= DS_2 \\ X_3 &= DS_3 = DS_4 = DS_5 = DS_6 \\ X_4 &= DS_F = DP_F = DB_F \\ X_5 &= DP_2 \\ X_6 &= DB_2 = DB_7 \\ X_7 &= DB_3 \\ X_8 &= DB_4 = DB_5 \\ X_9 &= DT \\ X_{10} &= DP_3 = DP_4 = DP_5 = DP_6. \end{aligned} \tag{16}$$

With regard to limited validity of some confluences it is helpful to devide them after transformation to following groups:

Group A

$$\begin{aligned} X_1 - X_2 + X_3 &= k0 \\ X_5 - X_{10} + X_4 &= k0 \\ X_6 - X_7 + X_4 &= k0 \\ X_2 - X_3 - X_4 &= k0 \\ X_7 - X_8 - X_6 &= k0 \\ X_5 - X_{10} &= k0. \end{aligned} \tag{17}$$

Group B1

$$\begin{aligned} X_6 - X_7 &= k0 \\ X_8 \qquad &= k0 \end{aligned} \tag{18}$$

Group B2

$$\begin{aligned} X_6 &= k0 \\ X_8 &= k0 \end{aligned} \tag{19}$$

Individual confluences

C1 $$X_{10} + X_4 + X_9 = k0 \tag{20}$$

C2 $$X_{10} - X_4 + X_9 = k0 \tag{21}$$

C3 $$X_{10} + X_4 - X_9 = k0 \tag{22}$$

C4 $$X_{10} - X_4 - X_9 = k0 \tag{23}$$

C5 $$X_4 = k0 \tag{24}$$

Non-linear dependences (see Fig. 4)

$$B_F = f(T)$$

is characterized by 5 linear sections (states s_3, s_4, s_5, s_6, s_7). In Fig. 5 are shown 4 states, in Fig. 3 two. Total number of various sets of confluences is 40. Nevertheless many of confluences are identical. For instance following confluence is valid for states s_3, s_5, s_7 (see Fig. 4)

$$DB_F = k0.$$

Therefore there are 10 various sets of confluences only. Set of 10 confluences is following

$$\begin{gathered} \text{A} - \text{B1} - \text{C1} \\ \text{A} - \text{B1} - \text{C2} \\ \text{A} - \text{B1} - \text{C3} \\ \text{A} - \text{B1} - \text{C4} \\ \text{A} - \text{B1} - \text{C5} \\ \text{A} - \text{B2} - \text{C1} \\ \text{A} - \text{B2} - \text{C2} \\ \text{A} - \text{B2} - \text{C3} \\ \text{A} - \text{B2} - \text{C4} \\ \text{A} - \text{B2} - \text{C5}. \end{gathered} \tag{25}$$

Couples of confluences B1 (see (*18*)) correspond to state s_1 (see Fig. 3) and confluences B2 correspond to state s_2. Individual confluences (see (*20*)–(*24*)) correspond to the following combinations of states (see Figs 4, 5):

C1 – s_6 and s_{10}
C2 – s_4 and s_9
C3 – s_4 and s_{10}
C4 – s_6 and s_9
C5 – (s_3 or s_7 or s_5) and (s_8 or s_{11}) .

Individual set of confluences are identified by means of combinations (*25*). Numbers of columns, in all tables, are consecutive numbers of qualitative variables X (see transformation (*16*)). Some parts of solution repeat. Therefore they are presented in blocks in Tables I–X. Letter x in the tables means that any qualitative value i.e. +, 0, – may be in relevant place (see (*1*)). In Table XI all solutions for four sets of confluences (A – B1 – C1, A – B1 – C2, A – B1 – C3, A – B1 – C4) are presented. Location of blocks from Tables I–VII is marked by consecutive number of block. Unnecessary columns, i.e. variables, are cut out.

Solution of confluence system A – B1 – C1 is shown in Table XII, system A – B1 – C5 in Table XIII and system A – B2 – C5 in Table XIV.

Table XII is valid also for systems A – B2 – C2, – C3, – C4. Only the ninth column is different. These columns are presented in Table XV.
Set of all possible qualitative solutions is not too transparent. Therefore it is helpful to make causal trees on basis of complete set of qualitative solutions.

TABLE I
Block 1 definition

	1	2	3	4
1	+	+	x	+
2	x	+	+	+
3	+	x	–	+
4	x	–	–	+
5	x	–	–	x
6	x	+	+	x
7	–	–	x	–
8	–	x	+	–
9	0	0	0	0

TABLE II
Block 2 definition

	1	2	3	4
1	–	–	x	–
2	x	–	–	–
3	–	x	+	–
4	x	+	+	–
5	x	–	–	x
6	x	+	+	x
7	+	+	x	+
8	+	x	–	+
9	0	0	0	0

TABLE III
Block 3 definition

	1	2	3	4
1	x	–	–	0
2	x	+	+	0
3	0	0	0	0

TABLE IV
Block 4 definition

	1	2	3	4	5	6	7	8	9	10
1	x	−	−	0	−	0	0	0	+	−
2	x	+	+	0	−	0	0	0	+	−
3	0	0	0	0	−	0	0	0	+	−
4	x	−	−	+	−	0	0	0	−	+
5	x	+	+	+	−	0	0	0	0	0
6	0	0	0	+	−	0	0	0	0	0
7	x	−	−	0	−	0	0	0	0	0
8	x	+	+	0	−	0	0	0	0	0
9	0	0	0	0	0	0	0	0	0	0

TABLE V
Block 5 definition

	8	9	10
1	0	x	−
2	0	x	−
2	0	x	−
4	0	x	−
5	0	+	−
6	0	+	−
7	0	+	−
8	0	+	−
9	0	+	−
10	0	x	+
11	0	x	+
12	0	x	+
13	0	x	+
14	0	−	+
15	0	−	+
16	0	−	+
17	0	−	+
18	0	−	+
19	0	0	0
20	0	0	0
21	0	0	0

TABLE VI
Block 6 definition

	8	9	10
1	0	x	−
2	0	x	−
3	0	x	−
4	0	x	−
5	0	−	−
6	0	−	−
7	0	−	−
8	0	−	−
9	0	−	−
10	0	x	+
11	0	x	+
12	0	x	+
13	0	x	+
14	0	+	+
15	0	+	+
16	0	+	+
17	0	+	+
18	0	+	+
19	0	0	0
20	0	0	0
21	0	0	0

TABLE VII
Block 7 definition

	1	8	10	9
1				−
2	B4			−
3				−
4				+
5				+
6				+
7				0
8				0
9				0

We search a causal tree with following set of primary qualitative values (*6*):

$$\begin{aligned} DS_5 &= k+ = X_3 \\ DP_5 &= k- = X_{10} \\ DP_F &= k- = X_4 \,. \end{aligned} \qquad (26)$$

Branching sequence (*11*) is

$$DS_1,\ DT_F,\ DB_7 \,. \qquad (27)$$

After transformation (*16*) this sequence is

$$X_1\ X_9\ X_6 \,. \qquad (28)$$

Causal tree is worked out for an intersection of states s_2, s_4, s_1 (see Figs 3, 4, 5). The final causal tree is shown in Fig. 7. If there is not qualitative solution for a path in the graph shown in Fig. 7, terminal point is marked by letter E (empty). In Table XVI all qualitative solutions are shown. Numbers in the first column are the numbers of terminal points of the tree, shown in Fig. 7.

One of the possible engineering interpretations of the graph shown in Fig. 7 is following. System leaves increasing quantity of substrate ($DS_5 = k+$). Simultaneously quantity of product in system outlet decreases ($DP_5 = k-$). Also generation of product decreases in fermentor ($DP_F = k-$). This situation is not economical.

Therefore we are interested in possible reasons and ways of neutralization of the situation. Various preferences (e.g. easy manipulation) specifies sequence of branching (see (*27*)).

Useful information may be derived from the causal tree (see Fig. 7) analysis. E.g. for

$$DB_7 = 0$$

TABLE VIII
Block 8 definition

	1	2	3
1	x	—	—
2	x	+	+
3	0	0	0

TABLE IX
Block 9 definition

	1	2	3
1	—	—	x
2	x	—	—
3	—	x	+
4	x	+	+

TABLE X
Block 10 definition

	1	2	3	*I*
1	+	+	x	
2	x	+	+	
3	+	x	—	
4	x	—	—	

TABLE XI

Sets of qualitative solutions for system of confluences A — B1 — C1, — C2, — C3, — C4 (see (*25*))

	A — B1 — C1					A — B1 — C2					A — B1 — C3					A — B1 — C4				
	4	5	6	7	10	4	5	6	7	10	4	5	6	7	10	4	5	6	7	10
1	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
2	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
3	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
4	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
5	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
6	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
7	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
8	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
9	1	—	—	—	5	2	—	—	—	5	1	—	—	—	6	2	—	—	—	6
10	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
11	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
12	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
13	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
14	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
15	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
16	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
17	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
18	2	+	—	—	5	1	+	—	—	5	2	+	—	—	6	1	+	—	—	6
19	3	0	—	—	5	3	0	—	—	5	3	0	—	—	6	3	0	—	—	6
20	3	0	—	—	5	3	0	—	—	5	3	0	—	—	6	3	0	—	—	6
21	3	0	—	—	5	3	0	—	—	5	3	0	—	—	6	3	0	—	—	6
22	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
23	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
24	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
25	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
26	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
27	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
28	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
29	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
30	1	—	+	+	5	2	—	+	+	5	1	—	+	+	6	2	—	+	+	6
31	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
32	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
33	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
34	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
35	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
36	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
37	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
38	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6

TABLE XI
(*Continued*)

	A — B1 — C1					A — B1 — C2					A — B1 — C3					A — B1 — C4				
	4	5	6	7	10	4	5	6	7	10	4	5	6	7	10	4	5	6	7	10
39	2	+	+	+	5	1	+	+	+	5	2	+	+	+	6	1	+	+	+	6
40	3	0	+	+	5	3	0	+	+	5	3	0	+	+	6	3	0	+	+	6
41	3	0	+	+	5	3	0	+	+	5	3	0	+	+	6	3	0	+	+	6
42	3	0	+	+	5	3	0	+	+	5	3	0	+	+	6	3	0	+	+	6
43	4				4	4				4	7				7	7				7
51	4				4	4				4	7				7	7				7

all terminal bindings are empty (E). See Fig. 7 nodes 2, 5, 8, 11, 14, 17, 20, 23 and 26. It means that value B_7 must be changed.

Idea of the second case study is basically different from the previous one, that has been formed less or more on basis of qualitative ideas about process behaviour. Qualitative model of anaerobic digestion is worked out on formal transcription of conventional model formed by a system of differential and algebraic equations. Basic model has been published[29] with sufficient commentary[30].

In paper[29] also numerical values of constant has been presented. Since numerical values are insignificant from qualitative model poit of view, the whole quantitative model is arranged to following sets of confluences:

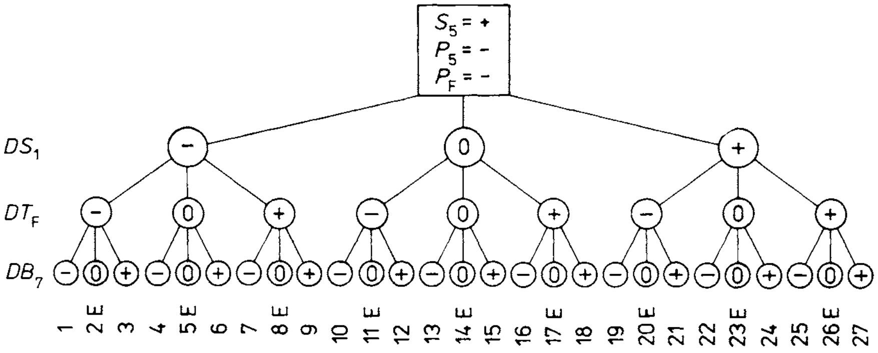

FIG. 7

Example of causal tree with following set PMQV (see Fig. 1): $s_5 = k+$, $P_5 = k-$, $P_5 = k-$

Liquid phase

$$X_1 = X_2 \, . \, X_3/X_4 \tag{29}$$

$$X_3 = X_5 \, . \, X_6/X_7 \tag{30}$$

$$X_7 = X_8 - X_2 \tag{31}$$

$$DX_8 = X_9/X_{10} \, . \, (X_{11} - X_8) \tag{32}$$

$$X_{12} = X_{13} \, . \, (X_{14} - X_6) \tag{33}$$

$$X_{14} = X_{15} \, . \, X_{16} \tag{34}$$

TABLE XII

Set of qualitative solutions for system of confluences A − B2 − C1

	1	2	3	4	5	6	7	8	9	10
1				−	−	0	−	−	+	−
2				−	−	0	−	−	+	−
3		B9		−	−	0	−	−	+	−
4				−	−	0	−	−	+	−
5				−	+	0	−	−	x	+
6		B9		−	+	0	−	−	x	+
7				−	+	0	−	−	x	+
8				−	+	0	−	−	x	+
9				+	−	0	+	+	x	−
10		B9		+	−	0	+	+	x	−
11				+	−	0	+	+	x	−
12				+	−	0	+	+	x	−
13		B9		+	+	0	+	+	−	+
14				+	+	0	+	+	−	+
15				+	+	0	+	+	−	+
16				+	+	0	+	+	−	+
17										
18										
19										
20					B4					
21										
22										
23										
24										
25										

TABLE XIII

Set of qualitative solutions for system of confluences A − B1 − C5

	1	2	3	4	5	6	7	8	9	10
1				0	−	−	−	0	x	−
2		B8		0	−	−	−	0	x	−
3				0	−	−	−	0	x	−
4				0	+	−	−	0	x	+
5		B8		0	+	−	−	0	x	+
6				0	+	−	−	0	x	+
7				0	0	−	−	0	x	0
8		B8		0	0	−	−	0	x	0
9				0	0	−	−	0	x	0
10				0	−	+	+	0	x	−
11		B8		0	−	+	+	0	x	−
12				0	−	+	+	0	x	−
13				0	+	+	+	0	x	+
14		B8		0	+	+	+	0	x	+
15				0	+	+	+	0	x	+
16				0	0	+	+	0	x	0
17		B8		0	0	+	+	0	x	0
18				0	0	+	+	0	x	0
19				0	−	0	0	0	x	−
20		B8		0	−	0	0	0	x	−
21				0	−	0	0	0	x	−
22				0	+	0	0	0	x	+
23		B8		0	+	0	0	0	x	+
24				0	+	0	0	0	x	+
25				0	0	0	0	0	x	0
26		B8		0	0	0	0	0	x	0
27				0	0	0	0	0	x	0

$$DX_{17} = X_9/X_{10} \,.\, (X_{18} - X_{17}) \qquad (35)$$

$$DX_6 = X_9/X_{10} \,.\, (X_{19} - X_6) + X_{12} + X_{20} + X_{21} \qquad (36)$$

$$X_{21} = X_9/X_{10} \,.\, (X_{22} - X_7) + DX_2 - DX_8 \,. \qquad (37)$$

Bio-phase

$$DX_{23} = X_9/X_{10} \,.\, (X_{24} - X_{23}) + X_{25} \,.\, X_{23} - X_{26} \,.\, X_{17} \qquad (38)$$

$$DX_2 = X_9/X_{10} \,.\, (X_{27} - X_2) - X_{25}/X_{29} \,.\, X_{23} \qquad (39)$$

$$X_{25} = X_{30}/(1 + X_{31}/X_1 + X_1/X_{32}) \qquad (40)$$

$$X_{20} = X_{33} \,.\, X_{25} \,.\, X_{23} \qquad (41)$$

$$X_{34} = X_{10}/X_{35} \,.\, X_{36} \,.\, X_{25} \,.\, X_{23} \qquad (42)$$

TABLE XIV

Set of qualitative solutions for system of confluences A — B2 — C5

	1	2	3	4	5	6	7	8	9	10
1	+	+	+	0	—	0	0	0	x	—
2	—	+	+	0	—	0	0	0	x	—
3	0	+	+	0	—	0	0	0	x	—
4	+	—	—	0	—	0	0	0	x	—
5	—	—	—	0	—	0	0	0	x	—
6	0	—	—	0	—	0	0	0	x	—
7	0	0	0	0	—	0	0	0	x	—
8	+	+	+	0	+	0	0	0	x	+
9	—	+	+	0	+	0	0	0	x	+
10	0	+	+	0	+	0	0	0	x	+
11	+	—	—	0	+	0	0	0	x	+
12	—	—	—	0	+	0	0	0	x	+
13	0	—	—	0	+	0	0	0	x	+
14	0	0	0	0	+	0	0	0	x	+
15	+	+	+	0	0	0	0	0	x	0
16	—	+	+	0	0	0	0	0	x	0
17	0	+	+	0	0	0	0	0	x	0
18	+	—	—	0	0	0	0	0	x	0
19	—			0	0	0	0	0	x	0
20	0	—	—	0	0	0	0	0	x	0
21	0	0	0	0	0	0	0	0	x	0

TABLE XV

Values of qualitative quantity X_9 for system of confluences A — B2 — C2, — C3, — C4 solution

	Confluences		
	C2	C3	C4
1	x	—	x
2	x	—	x
3	x	—	x
4	x	—	x
5	—	x	+
6	—	x	+
7	—	x	+
8	—	x	+
9	+	x	—
10	+	x	—
11	+	x	—
12	+	x	—
13	x	+	x
14	x	+	x
15	x	+	x
16	x	+	x

gas-phase

$$DX_{16} = -X_{37} \,.\, X_{10}/(X_{35} \cdot X_{38}) \,.\, X_{12} - X_{16}/X_{38} \,.\, X_{39} \tag{43}$$

$$X_{40} = -X_{10}/X_{35} \,.\, X_{12} \tag{44}$$

$$X_{39} = X_{40} + X_{34} + X_{41} \,. \tag{45}$$

In this system of confluences the quantities (*46*) are considered to be quantitative constants with qualitative values $k0$ and $k+$:

$$\begin{aligned} X_{35} &= \varrho_G = k+ \\ X_{27} &= s_0 = k+ \\ X_{11} &= z_0 = k+ \\ X_9 &= F = k+ \\ X_{19} &= [CO_2]_{Do} = k0 \\ X_{24} &= x_0 = k0 \end{aligned} \tag{46}$$

TABLE XVI

Sets of final qualitative solutions for causal tree from Fig. 7

	X1	X2	X3	X4	X5	X6	X7	X8	X9	X10
1	—	x	+	—	—	—	—	0	—	—
3	—	x	+	—	—	+	+	0	—	—
4	—	x	+	—	—	—	—	0	0	—
6	—	x	+	—	—	+	+	0	0	—
7	—	x	+	—	—	—	—	0	+	—
9	—	x	+	—	—	+	+	0	+	—
10	0	+	+	—	—	—	—	0	—	—
12	0	+	+	—	—	+	+	0	—	—
13	0	+	+	—	—	—	—	0	0	—
15	0	+	+	—	—	+	+	0	0	—
16	0	+	+	—	—	—	—	0	+	—
18	0	+	+	—	—	+	+	0	+	—
19	+	+	+	—	—	—	—	0	—	—
21	+	+	+	—	—	+	+	0	—	—
22	+	+	+	—	—	—	—	0	0	—
24	+	+	+	—	—	+	+	0	0	—
25	+	+	+	—	—	—	—	0	+	—
27	+	+	+	—	—	+	+	0	+	—

$$
\begin{aligned}
X_{22} &= [\mathrm{HCO}_3^-]_0 = k0\\
X_{18} &= [\mathrm{tox}]_0 = k0\\
X_2 &= s = k+\\
X_1 &= (hs) = k+\\
X_7 &= [\mathrm{HCO}_3^-] = k+\\
X_{23} &= x = k+\\
X_{16} &= p_{\mathrm{CO}_2} = k+\\
X_{25} &= \mu = k+\\
X_{34} &= Q_{\mathrm{CH}_4} = k+\\
X_{10} &= V = k+\\
X_{38} &= V_{\mathrm{G}} = k+\\
X_{30} &= \mu_{\mathrm{max}} = k+\\
X_{37} &= P_{\mathrm{T}} = k+\\
X_{13} &= k_{\mathrm{L}}a = k+\\
X_{31} &= K_{\mathrm{s}} = k+\\
X_{32} &= K_{\mathrm{i}} = k+\\
X_{29} &= Y_{\mathrm{x/s}} = k+\\
X_{33} &= Y_{\mathrm{CO}_2/\mathrm{x}} = k+\\
X_6 &= [\mathrm{CO}_2]_{\mathrm{D}} = k+\\
X_{36} &= Y_{\mathrm{CH}_4/\mathrm{x}} = k+\,.
\end{aligned}
$$

All other quantities are qualitative variables with following biotechnological interpretation (see refs[29,30]):

$$
\begin{aligned}
X_3 &= h^+\\
X_4 &= K_9\\
X_5 &= K_1\\
X_8 &= Z\\
X_{12} &= T_{\mathrm{G}}\\
X_{14} &= {}^2[\mathrm{CO}_2]_{\mathrm{D}}^* \qquad (47)\\
X_{15} &= k_{\mathrm{H}}\\
X_{17} &= [\mathrm{tox}]\\
X_{20} &= R_{\mathrm{B}}
\end{aligned}
$$

$$\begin{aligned} X_{21} &= R_C \\ X_{26} &= k_T \\ X_{39} &= Q \\ X_{40} &= Q_{CO_2} \\ X_{41} &= Q_{H_2O}. \end{aligned}$$

After qualitative rearrangement of confluences ((*29*)–(*45*)) and simultaneous utilization of qualitative values (*47*) we find that confluences (*31*), (*40*), and (*42*) are qualitatively identical (e.g. $k+ = k+$) and there is no reason to consider them further. After rearrangement we get set of confluences:

$$(29) \Rightarrow X_3/X_4 = k+ \tag{48}$$

$$(30) \Rightarrow X_3 = X_5 \tag{49}$$

$$(32) \Rightarrow DX_8 = k0 \tag{50}$$

$$(33) \Rightarrow X_{14} - X_{12} = k+ \tag{51}$$

$$(34) \Rightarrow X_{14} = X_{15} \tag{52}$$

$$(35) \Rightarrow DX_{17} = -X_{17} \tag{53}$$

$$(36) \Rightarrow DX_6 = k- + X_{12} + X_{20} + X_{21} \tag{54}$$

$$(37) \Rightarrow X_{21} = k- + DX_2 - DX_8 \tag{55}$$

$$(38) \Rightarrow DX_{23} = -X_{26} \cdot X_{17} \tag{56}$$

$$(39) \Rightarrow DX_2 = k0 \tag{57}$$

$$(41) \Rightarrow X_{20} - k+ \tag{58}$$

$$(43) \Rightarrow DX_{16} = -X_{12} - X_{39} \tag{59}$$

$$(44) \Rightarrow X_{40} = -X_{12} \tag{60}$$

$$(45) \Rightarrow X_{39} - X_{40} - X_{41} = k+. \tag{61}$$

System of confluences (*41*)–(*61*) is formed by three disjunctive subsets of confluences and by a co-ordination set of qualitative values. This co-ordination set is (*50*), (*57*), (*58*).

Rearranging confluence (*55*) and using values (*50*) and (*57*) we get

$$X_{21} = k- . \tag{62}$$

In such a way mentioned three disjunctive sets of confluences may be specified

$$X_3/X_4 = k+ \tag{63}$$

$$X_3 = X_5 \tag{64}$$

$$DX_{23} = -X_{17} \cdot X_{26} \tag{65}$$

$$DX_{17} = -X_{17} \tag{66}$$

$$X_{14} = X_{12} + k+ \tag{67}$$

$$X_{40} = -X_{12} \tag{68}$$

$$DX_{16} = -X_{12} - X_{39} \tag{69}$$

$$X_{41} = X_{12} + X_{39} + k- \tag{70}$$

$$DX_6 = X_{12} + X_{20} + k- \tag{71}$$

$$X_{15} = X_{14}. \tag{72}$$

Set of solutions of the first disjunctive set of confluences (*63*) and (*64*) is

Solution	X_3	X_4	X_5
1	$k+$	$k+$	$k+$
2	$k-$	$k-$	$k-$.

(*73*)

Set of solutions of the second disjunctive set of confluences (*65*) and (*66*) is

(*74*)

Solution	X_{17}	X_{26}	DX_{17}	DX_{27}
1	$k+$	$k+$	$k-$	$k-$
2	$k+$	$k0$	$k-$	$k0$
3	$k+$	$k-$	$k-$	$k+$
4	$k0$	$k+$	$k0$	$k0$
5	$k0$	$k0$	$k0$	$k0$
6	$k0$	$k-$	$k0$	$k0$
7	$k-$	$k+$	$k+$	$k+$
8	$k-$	$k0$	$k+$	$k0$
9	$k-$	$k-$	$k+$	$k-$.

Solution of the last system of confluences (*67*)–(*71*) follows simply from structure of those linear confluences. Qualitative quantities X_{12}, X_{39}, and X_{20} define qualitative values of quantities X_{14} (see (*67*)), X_{40} (see (*68*)), DX_{16} (see (*69*)) etc. Total number of solutions is 27 because three quantities (X_{12}, X_{39}, X_{20}) may acquire three qualitative values. Proper set of qualitative solutions is not presented because of its simplicity.

Information itself that the qualitative model disintegrates into three disjunctive models is useful and shows specific features of model. Causal tree may be set up within each subset of confluences.

CONCLUSIONS

Without formalization of common-sence reasoning further qualitative development of expert systems is impossible. It is related to natural language utilization for modelling of engineering systems. Application of natural language would bring a real qualitative to modelling. A problem is, how to make available "background of human experience" for computer. As a primitive example a descriptor "high" is presented. There is not an absolute value of this descriptor – high temperature in context with fermenter means something quite different than high temperature in context with a furnace for feed heating of crude oil primary distillation.

Using of engineering models in live language cannot be awaited in course of a few next years. Therefore a partial substitutions of live language must be intensively developed. One of them is a set of confluences.

However it strikes against a number of problems – sometimes almost of philosophical character[31]. It is in relation partly to present understanding of mathematical models (see e.g. refs[32,33]) and partly to a number of missunderstanding in conception of artificial intelligence as a whole and especially of expert systems (see e.g. ref.[34]).

Moreover it seems to be fairly promissing to incorporate some psychological concepts into engineering modelling[35]. All this makes a prediction of future development of formal tools very difficult. However it is quite certain that numerical model must be extended somehow to cover present practical needs.

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