AN INTEGRATION OF QUANTITATIVE AND QUALITATIVE KNOWLEDGE IN PROCESS ENGINEERING

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A value of a qualitative variable (derivative) can be positive, negative, or zero. Qualitative models are such models which contain qualitative variables only. Some parameters of an industrial process are measurable. Their time records are available. The main goal of this paper is to predict qualitative behaviour of all those variables which are not measured (cannot be measured) using time records of all such variables which are measured. Two case studies (damped oscillation, three reactor system) are given in full details.

Numerical mathematics and statistical analysis are the main formal tools how to solve various problems of process engineering (chemical engineering, bioengineering). However, many different industrial tasks cannot be solved by these formal tools.

The main reason is not e.g. numerical mathematics itself (nonlinearity, dimensionality). The problems under study are difficult to measure, very complex and ill-known. Many practical tasks are mostly solved not by a sophisticated formal tools but using an engineering common sense (diagnosis, fermentor control, reliability, pollution control, etc.).

Qualitative models seem to be a suitable formal specification of an engineering commonsense. Theory of qualitative modelling is available (see e.g. ref.[1]). Unfortunately generally accepted terminology does not exist. Several principially different concepts are used in qualitative modelling. Therefore the corresponding terminology depends heavily on the algorithms of modelling.

Moreover descriptions of qualitative algorithms require using of almost philosophical categories (see e.g. ref.[2]), in their very nature. Therefore their engineering interpretation is very vague.

What follows is a brief intuitive specification of the basic qualitative concepts[3].

BASIC CONCEPTS

Qualitative values are

+	–	increasing
0	–	constant
–	–	decreasing

A qualitative state is specified provided all its n qualitative variables

$$x_1, x_2, \ldots, x_n \tag{1}$$

are qualitatively described by a qualitative triplet

$$(X_i, DX_i, DDX_i), \tag{2}$$

where DX_i and DDX_i are the first qualitative and the second qualitative derivatives. A qualitative model

$$f(X_1, X_2, \ldots, X_n) = 0 \tag{3}$$

has m qualitative solutions. The j-th qualitative state is[1,2]

$$((X_1, DX_1, DDX_1), \ldots, (X_n, DX_n, DDX_n))_j$$

$$j = 1, 2, \ldots, m\,. \tag{4}$$

A simple commonsence analysis gives the following transition

$$\begin{array}{ccc} X, DX, DDX & & X, DX, DDX \\ (+ \quad 0 \quad +) & \rightarrow & (+ \quad + \quad +) \end{array} \tag{5}$$

A systematic study of n dimensional transitions enables development of a state graph. Nodes of the state graph are qualitative states and edges are possible transitions among the states[4].

There are already algorithms for the development of the state graph[4]. A realistic qualitative model gives more than 1 000 qualitative states. Consequently there are more than 3 000 transitions. A simple technology (reactor, separator) can have more than 30 000 transitions.

An engineering interpretation of such graphs is very time-consuming. Probability of human errors is relatively very high.

Therefore any simplification of the state graph is desirable. The obvious way how to decrease the number of edges and nodes is to use any additional quantitative knowledge, which is available.

The main practical problem which must be solved is an integration of qualitative models and quantitative measurements (records). A general methodology how to solve this task does not exist yet. A special algorithm is proposed in this paper. It accepts quantitative (time) records of some variables as the additional quantitative knowledge.

Even integration of such special quantitative knowledge and a general qualitative model seems to be very useful for solution of very important practical problems e.g. control, diagnosis, experiment planning, plant operator intelligent guide.

QUALITATIVE MODEL

Deep knowledge is closely connected to the laws of nature. Deep knowledge is typically represented by mass and energy conservation law. Both deep and shallow knowledge can be given in both analytical and/or verbal form. Polynom is a typical representative of shallow knowledge.

Figure 1 shows a mixer of the streams No. 1 and No. 2. The mass flow in stream No. i is q_i. A balance equation is

$$q_1 + q_2 = q_3 . \qquad (6)$$

Qualitative variables are marked by capital letters therefore the balance equation (*6*) transformed into the confluence (qualitative equation, for details see ref.[2]) is

$$Q_1 + Q_2 = Q_3 . \qquad (7)$$

Differentiating this equation gives

$$DQ_1 + DQ_2 = DQ_3 . \qquad (8)$$

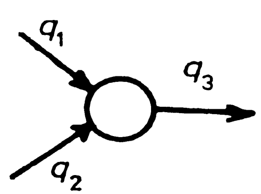

FIG. 1
Stream mixer

Let us suppose that the third flowrate increases

$$DQ_3 = + . \tag{9}$$

The confluence system (*8*), (*9*) gives five qualitative solutions:

Sol.	DQ_1	DQ_2	DQ_3
1	+	+	+
2	+	–	+
3	–	+	+
4	+	0	+
5	0	+	+

(*10*)

Any algebraical qualitative operation is specified provided the resulting triplet (*2*) is given. An example is addition

		input DQ_1 +	0	–
	+	+	+	?
input DQ_2	0	+	0	–
	–	?	–	–

(*11*)

The character "?" in matrix (*11*) means + or 0 or – . The same matrix is valid for the second derivative as well. The matrix (*11*) is so transparent that it does not require any additional explanation.

A study of qualitative problems solutions is not the aim of this paper. These methods can be found e.g. in refs[1 – 4]. This paper deals exclusively with deep and shallow knowledge integration.

STATE GRAPH

To demonstrate a simplicity of the basic algorithm for development of state graphs let us suppose that $n = 1$ (3). The one dimensional transition graph can have two types of transition, namely transition U and D.

U (Unknown) transition is a transition which may occure, because of the unknown third derivative. Let us suppose that instead of the triplet (*2*) the 4-plet

$$X, \mathrm{D}X, \mathrm{DD}X, \mathrm{DDD}X \quad (12)$$

is used. DDDX is the third qualitative derivative.

A simple commonsence analysis gives

$$(+ + + +) \rightarrow (+ + + +)$$
$$(+ + + 0) \rightarrow (+ + + 0)$$
$$(+ + + -) \rightarrow (+ + 0 -) . \quad (13)$$

Three transitions with the known third derivative are represented by two possible transitions with the unknown third derivative

$$(+ + +) \rightarrow (+ + +)$$
$$(+ + +) \rightarrow (+ + 0) . \quad (14)$$

The example (*14*) is just a part of the complete set of U-transitions.

D (Derivative) transition is the transition which is based on an understanding of derivative as e.g.

$$(+ + -) \rightarrow (+ 0 -)$$
$$(+ - +) \rightarrow (0 - +)$$
$$(+ - +) \rightarrow (+ + +) . \quad (15)$$

The reasoning used for D-transition (*15*) is very simple. For example the negative second derivative will decrease the positive first derivative.

The qualitative state graph is an oriented graph where every node is one qualitative state (*4*). Every edge is induced by D and U transitions between the two nodes.

DEMONSTRATIVE EXAMPLE

A qualitative model of the damped oscillation is chosen as a demonstrative example. The reason is that it is well known and relatively simple. The conventional model (set of differential equations) is as follows[5]

$$x2' = -k2 * x2 - k1 * x1$$
$$x1' = x2 . \quad (16)$$

The quantitative solution of the oscillating loop i.e. evaluation of the variables $v1$ to $v5$ with

$$\begin{aligned} v1 &= x1 \\ v2 &= x2 \\ v3 &= x2' \\ v4 &= -k1 * x1 \\ v5 &= -k2 * x2 \end{aligned} \tag{17}$$

was performed by the Runge–Kutta fourth order method.

Two quantitative alternatives were studied:

(i) $k1 = 4;\ k2 = 0.8$ i.e. oscilating loop

(ii) $k1 = 1;\ k2 = 2$ i.e. loop at the aperiodic limit. (*18*)

The Eq. (*16*) of the oscillating loop may be transformed into the confluences

$$\begin{aligned} \mathrm{D}X2 + k2 * X2 + k1 * X1 &= 0 \\ \mathrm{D}X1 &= X2 . \end{aligned} \tag{19}$$

There are two qualitative variables $X1$, $X2$ (see $n = 2$, (Eq. (*1*)) and two qualitative constants $k1 = k2 = +$. For example $\mathrm{D}X2$ is a qualitative description of $x2'$.

The set of Eqs (*19*) can be transformed into a diagram (see Fig. 2). A correspondence of the set of Eqs (*19*) and Fig. 2 gives an explanation of all blocks.

The set of all qualitative states of the loop (see Eqs (*19*)) is in Table I and the set of possible transitions among them (see Fig. 3) were obtained.

The number of different qualitative states is (see 4-flet (Eq. (*12*)), Table I) $m = 45$.

Numbers of the nodes in Fig. 3 are the numbers of the qualitative states in Table I.

A qualitative interpretation of any quantitative simulation represents actually a path in the state graph i.e. a quantitative simulation is a chronological sequence of some qualitative states (*4*). All possible sequences are subgraphs of the state graph. It means that a qualitative description of any qualitative "dynamic behaviour" of the model (*14*) for any numerical values of constants $k1$, $k2$ (see Eqs (*18*)) must be covered by the corresponding state subgraph.

Qualitative interpretation of a variable record is very straightforward and simple. See Fig. 4, where this transformation is given.

TABLE I
The complete list of all qualitative states of the loop

State No.	*V1*	*V2*	*V3*	*V4*	*V5*
1	+ + −	+ − +	− + +	− − +	− + −
2	+ + −	+ − +	− + 0	− − +	− + −
3	+ + −	+ − +	− + −	− − +	− + −
4	+ + −	+ − 0	− 0 +	− − +	− + 0
5	+ + −	+ − −	− − +	− − +	− + +
6	+ 0 −	0 − +	− + +	− 0 +	0 + −
7	+ 0 −	0 − +	− + 0	− 0 +	0 + −
8	+ 0 −	0 − +	− + −	− 0 +	0 + −
9	+ − +	− + +	+ + −	− + −	+ − −
10	+ − +	− + 0	+ 0 −	− + −	+ − 0
11	+ − +	− + −	+ − +	− + −	+ − +
12	+ − +	− + −	+ − 0	− + −	+ − +
13	+ − +	− + −	+ − −	− + −	+ − +
14	+ − 0	− 0 +	0 + −	− + 0	+ 0 −
15	+ − −	− − +	− + +	− + +	+ + −
16	+ − −	− − +	− + 0	− + +	+ + −
17	+ − −	− − +	− + −	− + +	+ + −
18	0 + −	+ − +	− + +	0 − +	− + −
19	0 + −	+ − +	− + 0	0 − +	− + −
20	0 + −	+ − +	− + −	0 − +	− + −
21	0 + −	+ − 0	− 0 +	0 − +	− + 0
22	0 + −	+ − −	− − +	0 − +	− + +
23	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
24	0 − +	− + +	+ + −	0 + −	+ − −
25	0 − +	− + 0	+ 0 −	0 + −	+ − 0
26	0 − +	− + −	+ − +	0 + −	+ − +
27	0 − +	− + −	+ − 0	0 + −	+ − +
28	0 − +	− + −	+ − −	0 + −	+ − +
29	− + +	+ + −	+ − +	+ − −	− − +
30	− + +	+ + −	+ − 0	+ − −	− − +
31	− + +	+ + −	+ − −	+ − −	− − +
32	− + 0	+ 0 −	0 − +	+ − 0	− 0 +
33	− + −	+ − +	− + +	+ − +	− + −
34	− + −	+ − +	− + 0	+ − +	− + −
35	− + −	+ − +	− + −	+ − +	− + −
36	− + −	+ − 0	− 0 +	+ − +	− + 0
37	− + −	+ − −	− − +	+ − +	− + +
38	− 0 +	0 + −	+ − +	+ 0 −	0 − +
39	− 0 +	0 + −	+ − 0	+ 0 −	0 − +
40	− 0 +	0 + −	+ − −	+ 0 −	0 − +
41	− − +	− + +	+ + −	+ + −	+ − −
42	− − +	− + 0	+ 0 −	+ + −	+ − 0
43	− − +	− + −	+ − +	+ + −	+ − +
44	− − +	− + −	+ − 0	+ + −	+ − +
45	− − +	− + −	+ − −	+ + −	+ − +

The qualitative interpretation of quantitative simulation (i) and (ii) (see Eqs (*18*)) is used to eliminate some transitions from the state graph. A commonsence reason on which this elimination is based is very simple. The records of variables *vi*, $i = 1, 2, \ldots 5$ (see Eqs (*16*) and (*17*)) are known (measurement or numerical solution of the differential equations).

They can be therefore used to eliminate such qualitative states which cannot occure. The result of this elimination is a qualitative description of a dynamic behaviour of these variables which are not measured (see Table II for simulation (*18*) (i) and Table III for simulation (*18*) (ii)).

This problem is very important in e.g. biotechnology and pharmacy, where it is often impossible to measure certain variables. Suitable sensors are not available.

The qualitative states listed in the Tables II and III were compared with the qualitative model solution and numbered in accordance with the Table I (the right edge column in the Tables II and III). The resulting qualitative states sequences were compared with the state graph (see Fig. 3).

The nodes of the subgraph representing the type (i) sequence are represented with the crossed circles (see Fig. 3). The nodes of the subgraph representing the type (ii) sequence are represented by the double circles with a line (see Fig. 3).

The comparison indicates that:

- all the qualitative states obtained by the analysis of the numerical model solution are listed in the qualitative model solution list;
- qualitative state graph obtained by the analysis of the numerical simulation is a subgraph of the qualitative model simulation graph.

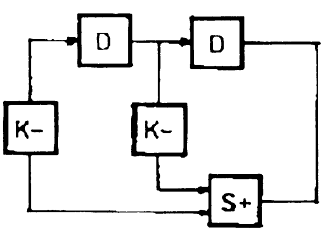

FIG. 2
Qualitative oscillating loop

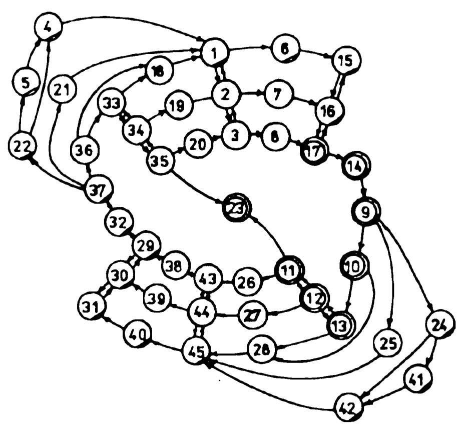

FIG. 3
The complete state graph of the loop

TABLE II
List of qualitative states for the loop simulation (i). The corresponding states of the state graph (Table I) are listed in the right edge column

Time	*V*1	*V*2	*V*3	*V*4	*V*5	State No.
0.0	+ 0 0	0 0 0	0 0 0	− 0 0	0 0 0	
	+ − −	− − +	− + +	− + +	+ + −	15
0.7	+ − −	− − +	− + 0	− + +	+ + −	16
	+ − −	− − +	− + −	− + +	+ + −	17
0.8	+ − 0	− 0 +	0 + −	− + 0	+ 0 −	14
	+ − +	− + +	+ + −	− + −	+ − −	9
0.9	0 − +	− + +	+ + −	0 + −	+ − −	24
	− − +	− + +	+ + −	+ + −	+ − −	41
1.5	− − +	− + 0	+ 0 −	+ + −	+ − 0	42
	− − +	− + −	+ − −	+ + −	+ − +	45
1.6	− 0 +	0 + −	+ − −	+ 0 −	0 − +	40
	− + +	+ + −	+ − −	+ − −	− − +	31
2.3	− + +	+ + −	+ − 0	+ − −	− − +	30
	− + +	+ + −	+ − +	+ − −	− − +	29
2.4	− + 0	+ 0 −	0 − +	+ − 0	− 0 +	32
	− + −	+ − −	− − +	+ − +	− + +	37
2.5	0 + −	+ − −	− − +	0 − +	− + +	22
	+ + −	+ − −	− − +	− − +	− + +	5
3.1	+ + −	+ − 0	− 0 +	− − +	− + 0	4
	+ + −	+ − +	− + +	− − +	− + −	1
3.2	+ 0 −	0 − +	− + +	− 0 +	0 + −	6
	+ − −	− − +	− + +	− + +	+ + −	15
3.9	+ − −	− − +	− + 0	− + +	+ + −	16

TABLE III
List of qualitative states for the loop simulation (ii). The corresponding states of the state graph (Table I) are listed in the right edge column

Time	*V*1	*V*2	*V*3	*V*4	*V*5	State No.
	− 0 0	0 0 0	0 0 0	− 0 0	0 0 0	
0.0	+ − −	− − +	− + −	− + +	+ + −	17
1.1	+ − 0	− 0 +	0 + −	− + 0	+ 0 −	14
	+ − +	− + +	+ + −	− + −	+ − −	9
2.1	+ − +	− + 0	+ 0 −	− + −	+ − 0	10
	+ − +	− + −	+ − −	− + −	+ − +	13
4.0	+ − +	− + −	+ − 0	− + −	+ − +	12
	+ − +	− + −	+ − +	− + −	+ − +	11
	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0	23

These conclusions confirm the solutions given in Tables II and III. For example the value of the variable $v3$ cannot decrease in the states 15, 16, 17 and must decrease in the states 29, 30, 31.

Rather often the total number of qualitative variables is large. However, an engineer is not interested in all variables all the time. Therefore some variables can be uninteresting from the specific point of view.

A "point of view" can be represented as a choice of important and unimportant variables. An unimportant variable is such variable that cannot discriminate. Two qualitative states are identical even if they have different values of the unimportant variables.

If we declare the derivative $DV3$ to be unimportant, the state graph (see Fig. 3) is transformed into the state graph given in Fig. 5 and the list in Table I is transformed into the list given in Table IV.

CASE STUDY

The model of three CSTR's in series[5] was chosen as the chemical engineering application. A closed-loop three-CSTR process is shown on Fig. 6. Its conventional model is

$$\frac{dC_{A1}}{dt} = \frac{1}{\tau} - (C_{A0} - C_{A1}) - k\,C_{A1}$$

$$\frac{dC_{A2}}{dt} = \frac{1}{\tau} - (C_{A1} - C_{A2}) - k\,C_{A2}$$

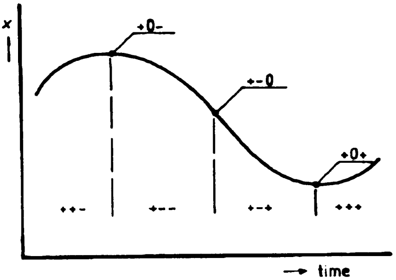

FIG. 4
Qualitative transformation example

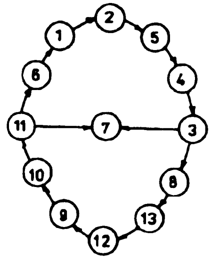

FIG. 5
The reduced state graph of the loop

TABLE IV
The reduced list of qualitative states of the loop. The corresponding states of the complete state graph (Table I) are listed in the left edge column

State No.	*V1*	*V2*	*V3*	*V4*	*V5*
1 (1 – 5)	+ + –	+ – ?	– ? ?	– – +	– + ?
2 (6 – 8)	+ 0 –	0 – +	– + ?	– 0 +	0 + ?
3 (9 – 13)	+ – +	– + ?	+ ? ?	– + –	+ – ?
4 (14)	+ – 0	– 0 +	0 + –	– + 0	+ 0 –
5 (15 – 17)	+ – –	– – +	– + ?	– + +	+ + –
6 (18 – 22)	0 + –	+ – ?	– ? ?	0 – +	– + ?
7 (23)	0 0 0	0 0 0	0 0 0	0 0 0	0 0 0
8 (24 – 28)	0 – +	– + ?	+ ? ?	0 + –	+ – ?
9 (29 – 31)	– + +	+ + –	+ – ?	+ – –	– – +
10 (32)	– + 0	+ 0 –	0 – +	+ – 0	– 0 +
11 (33 – 37)	– + –	+ – ?	– ? ?	+ – +	– + ?
12 (38 – 40)	– 0 +	0 + –	+ – ?	+ 0 –	0 – +
13 (41 – 45)	– – +	– + ?	+ ? ?	+ + –	+ – ?

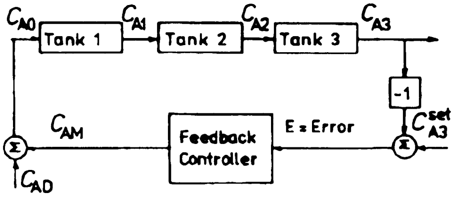

FIG. 6
The three CSTR's model

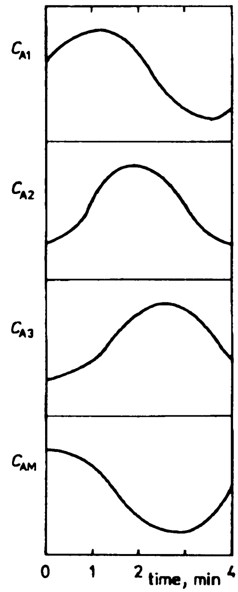

FIG. 7
Course of variables in three CSTR's model

$$\frac{dC_{A3}}{dt} = \frac{1}{\tau} - (C_{A2} - C_{A3}) - k\,C_{A3}$$

$$C_{AM} = 0.4 + k_c\,(E + \frac{1}{\tau}E_{(t)}\,dt)\,. \qquad (20)$$

TABLE V
List of qualitative states for three CSTR's simulation

State No.	C_{A1}	C_{A2}	C_{A3}	C_{AM}
1	+ − +	+ − −	+ + −	+ − +
2	+ − +	+ − −	+ 0 −	+ − +
3	+ − +	+ − −	+ − −	+ − +
4	+ − +	+ − −	+ − −	+ 0 +
5	+ − +	+ − −	+ − −	+ + +
6	+ − +	+ − 0	+ − −	+ + +
7	+ − +	+ − +	+ − −	+ + +
8	+ 0 −	+ − +	+ − −	+ + +
9	+ + +	+ − +	+ − −	+ + +
10	+ + +	+ − +	+ − 0	+ + +
11	+ + +	+ − +	+ − +	+ + +
12	+ + +	+ − +	+ − +	+ + 0
13	+ + +	+ − +	+ − +	+ + −
14	+ + +	+ 0 −	+ − +	+ + −
15	+ + +	+ + +	+ − +	+ + −
16	+ + 0	+ + +	+ − +	+ + −
17	+ + −	+ + +	+ − +	+ + −
18	+ + −	+ + +	+ − +	+ 0 −
19	+ + −	+ + +	+ − +	+ − −
20	+ + −	+ + +	+ 0 +	+ − −
21	+ + −	+ + +	+ + +	+ − −
22	+ + −	+ + 0	+ + +	+ − −
23	+ + −	+ + −	+ + +	+ − −
24	+ 0 −	+ + −	+ + +	+ − −
25	+ − −	+ + −	+ + +	+ − −
26	+ − −	+ + −	+ + 0	+ − −
27	+ − −	+ + −	+ + −	+ − −
28	+ − −	+ + −	+ + −	+ − 0
29	+ − −	+ + −	+ + −	+ − +
30	+ − −	+ 0 −	+ + −	+ − +
31	+ − −	+ − −	+ + −	+ − +
32	+ − 0	+ − −	+ + −	+ − +

This system was qualitatively studied and the complete set of qualitative states and the state graph were obtained. This complete graph, however, is very extensive and therefore it cannot be presented here.

The quantitative records of C_{A3}, C_{AM} (ref.[5], p. 143) are used as the additional information and may be completed by the qualitative time charts of C_{A1}, C_{A2} (Fig. 7).

The reduced graph is cyclic. The set of its nodes i.e. actually possible qualitative states is listed in Table V.

In the time interval 0 to 4 min the qualitative cycle of Table V is followed in the course of the qualitative states numbered 21 to 32 and 1 to 13. For comparison consider the qualitative course of C_{A3}, C_{AM} and Table V.

LIST OF SYMBOLS

$k1$, $k2$	constants of the oscillating loop
k_c	feedback controller gain
m	number of different qualitative states in a model
$x1$, $x2$	oscillating loop state variables
C_{A0}	concentration to the first stage of three CSTR's
C_{A1}	concentration to the second stage of three CSTR's
C_{A2}	concentration to the third stage of three CSTR's
C_{A3}	outlet flow concentration of CSTR's model
C_{AM}	manipulative concentration of CSTR's model
C_{AD}	disturbance concentration of CSTR's inlet flow
C_{A3}^{set}	set-point value of C_{A3}
E	error, $E = C_{A3}^{set} - C_{A3}$
τ	feedback reset time

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