

**Abstract:** This paper presents a causal simulation method for incompletely known dynamic systems in process engineering. The causal model of a process is represented as both a causal network of interacting elementary dynamic systems, called qualitative automata, influencing one another, and a set of qualitative constraints linking possibly several of such automata. Associated with each influence is a weight which expresses its sensitivity. A procedure is presented which allows us to generate fuzzy weights from the relative order of magnitude relations between them. Formulae preserving non-linearities and fulfilling some relevant requirements are provided to compute net influences on extensive variables as well as on intensive ones. Finally an algorithm is given for simulating the causal model, and an example application to a fed-batch fermentation process is presented.

## 1 Introduction

One of the most difficult tasks to deal with while controlling and monitoring a dynamic process is to predict its behavior. The problem is that some of the process variables may be difficult to measure on-line, or are not measured at all (e.g. simply because appropriate sensors are not available). Control theories provide tools for state prediction and estimation when precise quantitative models in terms of equations and functions are available. Meanwhile in process engineering, accurate equational and functional quantitative models are not often available because of the complexity of the systems to cope with. For instance in biotechnology, 1) the processes usually contain variables varying rapidly in time, 2) the process dynamics is non-linear and not reproducible, 3) the interactions between the process variables and parameters are not all known, 4) the processes are subject to permanent inner disturbances. Therefore, most of engineering processes are incompletely known.

To endow computer systems with abilities to reason about qualitative models, work in Qualitative Physics (QP) [16] has focused on qualitative simulation [6,9] of dynamic systems, that is, qualitative differential equation (QDE) based reasoning. The advantage of QDE-based simulators is the ability to yield all the possible qualitative behaviors of any incompletely known, or described, dynamic system using much less computational intensive algorithms than those required by numerical simulation. However, they suffer from some limitations mainly related to the weakness of their expressive power, the time-scale abstraction they bear in themselves, and to the fact that they are only concerned with real-valued variables and remain silent about pure symbolic variables. Causal reasoning - reasoning based on the causal interactions between the variables and parameters of a system - may be seen as a way to overcome some of the shortcomings of QDE-based systems in that 1) it does not require having differential equations, 2) it deals with directed relationships, 3) it may cope with time explicitly which makes it possible to take into account influence delays and durations, 4) it can provide a framework for knowledge elicitation since experts and engineers use concepts of causality for the interpretation, prediction and explanation of dynamic systems.

Causal simulation (i.e. the simulation of dynamic systems based on the causal relationships among their variables and parameters) is necessary for reasoning about non mathematically formalized dynamic processes such as those often encountered in biotechnology, chemistry, ecology, physiology etc... and in which causality is the guideline. Meanwhile, attention has only been

paid to it episodically. Guerrin [7] proposes ways to combine states of variables influencing a single one using qualitative operators. Leyval and Gentil [10], Vescovi [15], and Djerroud et al. [4] combine the trends of variables using classical summation operator thus neglecting the use of influence weights and the capability to approximate non-linear relationships. Schmoldt [13] has built a causal simulation formalism which seems to be too specific for ecophysiological processes; furthermore, although he associates weights to influences and takes into account non-linearities, the computational complexity of his method makes it cumbersome for real-time applications in process engineering. D'Ambrosio [3] has proposed an algorithm for reducing the undecidability during influence combination in qualitative process theory [6] using linguistic descriptions of influence sensitivities; but his method requires having the necessary problem specific information to combine influences properly, and like Schmoldt, he neither provides any formal means to determine influence weights of variables, nor to check the consistency of a set of influences weights when they are given by experts. Another aspect which has been neglected in previous approaches is that they do not distinguish extensive variables from intensive ones. Assume the marginal influences of two variables on the length (an *extensive* variable) of a metal bar to be respective increases of its value by 1 *cm* and 2 *cm* with the same influence weight, then the net (total) influence of those variables on the length is 3 *cm*. On the contrary, if the marginal influences of the two variables on the temperature (which is an *intensive* variable) of the metal bar are increases by 1°*F* and 2°*F*, then the net influence will never be 3°*F*, but less, whatever the influence weights are. Hence, the net influence on an extensive variable is the algebraic weighted sum of the individual influences whereas the net influence on an intensive variable is a mean of the individual influences.

This paper proposes a method for causal simulation of incompletely known dynamic processes which addresses most of the limitations of the existing ones. The method describes a part of the CA-EN (CAusal ENgine) system which is aimed at supervising incompletely known dynamic engineering processes. Section 2 presents an insight into the modeling formalism which is completely described in [1]; Section 3 proposes a method for computing fuzzy influence weights from linguistic description of their relative orders of magnitude; section 4 is concerned with weighted influence combination, and an algorithm for propagating influences through the causal network of the process variables, section 5 presents an example application of the method to a fed-batch fermentation process, and the last section concerns a discussion of the method.

## 2 The modeling formalism

The process variables are either numeric (real-valued) or symbolic-valued. The value set of a numeric variable is a real interval or the whole real line; that of a symbolic variable is assumed to contain a finite number of elements. Whilst numeric variables are measured when there are appropriate sensors, and that their respective value sets are partitioned into finite numbers of intervals according to the context of use, symbolic variables are observed. We refer to *quality space* for a numeric variable, the partition of its value set; the quality space of a symbolic variable equals its value set. The *variation space* of a numeric variable is the partition of its change value set (i.e. the set of all the possible change values during a temporal unit) into a finite number of intervals. Symbolic variables have no variation spaces. Qualitatively, the behavior of a process variable is a sequence of discrete states which are either real intervals (if the variable is real-valued) or symbolic values. Therefore, the commonsense perception of a process variable is on one hand that of an automaton moving from an interval or a discrete value to another, and on the other hand the knowledge that is necessary to reason about its behavior with regard to its interactions with other variables. That suggests that we assign an elementary dynamic system, a *qualitative automaton* (or *q-automaton* for short), to each process variable and to the knowledge which is needed to reason about the behavior of the variable.

Conceptually, a q-automaton consists of a *quality space*, a *variation space* and an influence

combining function if the q-automaton is numeric, a transition function that represents the dynamics of the q-automaton in the absence of any external effect, an output function, and a state updating function.

A process is represented as two levels of constraints: *local constraints* and *global constraints*. Local constraints are causal relations involving two q-automata. There are two kinds of causal relations: one is concerned with cause-effect interactions among numeric q-automata only (e.g. if the amount of liquid in the tank increases then the pressure at the bottom of the tank increases as well) and the other is concerned with information about q-automata (e.g. the color of the liquid informs us about the concentration rate of a certain chemical product in it, but the influence rather goes from the concentration rate to the color). We refer to the former relations as *influence-based relations*, and the latter as *information-based relations*. A global constraint is a numeric or qualitative equation involving possibly several q-automata.

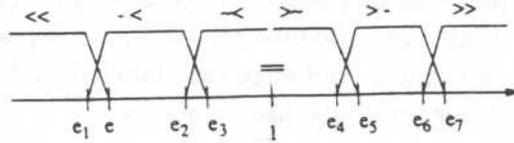


Fig.1: Fuzzy extension to order of magnitude formalism.  
 $e < 0.4656$ ;  $e_1 = e/(1+e)$ ;  $e_2 = (1+e)^2$ ;  $e_3 = (1+e)^3$ ;  
 $e_4 = 1/e_3$ ;  $e_5 = 1/e_2$ ;  $e_6 = 1/e$ ;  $e_7 = 1/e_1$ .

O(M) relation	Verbal explanation
$A \ll B$	A is much smaller than B
$A \prec B$	A is moderately smaller than B
$A \prec B$	A is slightly smaller than B
$A = B$	A is exactly equal to B
$A \succ B$	A is slightly larger than B
$A \succ B$	A is moderately larger than B
$A \gg B$	A is much larger than B

Table 1: Primitive relations of the order of magnitude formalism

An influence-based relation is described by means of predicate  $I_{\alpha}^{+}(X, Y, c, w, d, p)$ , or  $I_{\alpha}^{-}(X, Y, c, w, d, p)$ , where:  $X$  is the influencing q-automaton;  $Y$  the influenced q-automaton;  $c$  the activation precondition of the causal relation (the influence from  $X$  to  $Y$  is said to be activated whenever  $c$  holds);  $w$  is the weight of the influence of  $X$  on  $Y$ ;  $d$  is a real number representing the delay of the influence;  $p$  is a real number representing the influence duration, or equals  $\infty$  if the influence holds permanently. Actually, weight  $w$  is expressed by means of its relative orders of magnitude with respect to other weights of influences on  $Y$  in the fuzzy counterpart of the O(M) formalism (fig. 1 and table 1) (in the O(M) formalism, if  $r$  is an order of magnitude relation, and  $a$  and  $b$  two quantities, then  $(a \ r \ b)$  if, and only if  $(a/b \ r \ 1)$ ) [11]; that allows it to compute the fuzzy value of  $w$  accordingly as presented in the next section.

With reference to fig. 1, consistency in the partitioning of the real-line requires satisfying the constraint  $e < e_2$ , for  $e$  being the largest real supposed to be much smaller than 1, it must not be slightly smaller than 1, hence  $e < e_2$ . Satisfying the inequality  $e < e_2$  leads to  $e < 0.4656$ .

Predicate  $I_{\alpha}^{+}(X, Y, c, w, d, p)$  (resp.  $I_{\alpha}^{-}(X, Y, c, w, d, p)$ ) holds if, and only if  $X$  influences positively (resp. negatively)  $Y$ , where  $\alpha \in \{0, 1, 2, 3\}$  is the relative variation rate;  $\alpha = 0$  if  $Y$  increases (resp. decreases) in the same proportion as  $X$ ;  $\alpha = 1$  if  $Y$  increases (resp. decreases) slightly more than  $X$ ;  $\alpha = 2$  if  $Y$  increases (resp. decreases) moderately more than  $X$ ;  $\alpha = 3$  if  $Y$  increases (resp. decreases) much more than  $X$ . The relative order of magnitude of the variation of  $Y$  with respect to that of  $X$  are phrased in the O(M) formalism.

An information-based relation is represented as  $I(X, Y)$  where  $X$  is the informing q-automaton and  $Y$  a numeric q-automaton that  $X$  informs about. The description of such a relation is expressed by means of a mapping from the quality space of  $X$  to that of  $Y$ . Whilst influence-based relation only link numeric q-automata, information-based relations concern any type of q-automata. Information-based relations take precedence over influence-based relations.

A global constraint is a functional numeric constraint relating possibly more than two process

variables associated with interval domains. In other words, a global constraint is any numeric equation (in the classical sense) in which each unknown is supposed to take on interval values.

### 3 Generating fuzzy weights of influences

Experience acquired through collaboration with process experts indicates that these experts estimate net influences on variables using the relative orders of magnitude between individual influence weights rather than their pure numeric values; furthermore, they hesitate to provide numeric weights to influences when they are asked to. However to automate the weighted influence computation, it is convenient that weights be numeric or numeric-like. The hesitation of experts stems from the fact that weights may have hazy values. Hence, we propose a method to attribute fuzzy values to weights from the linguistic description of their relative orders of magnitude.

Let  $Y$  be a  $q$ -automaton, and  $X_1, \dots, X_n$  be  $n$  numeric  $q$ -automata influencing  $Y$  with respective influence weights  $w_1, \dots, w_n$  through influence-based relations. The linguistic description of orders of magnitude of the weights is a set of pairwise link between these weights (e.g. if the influence weight  $w_i$  of  $X_i$  on  $Y$  is much smaller than the influence  $w_j$  of  $X_j$  on  $Y$ , we write  $w_i \ll w_j$ ). That gives rise to a graph whose nodes are weights, and edges are labeled by fuzzy  $O(M)$  relations (because of the symmetry of  $O(M)$  relations, we only use relations  $\ll$ ,  $- <$ ,  $\sim <$ , and  $=$  to express relative orders of magnitude between weights). To compute the absolute values of the weights we assume the graph to be connex and that there exists a weight  $w_{max}$  such that for any weight  $w_i$ , there exists a path in the graph from  $w_i$  to  $w_{max}$ . Therefore the graph must be an upper semi-lattice for which  $w_{max}$  is the greatest element. We term such a lattice as the *weight lattice* associated with  $q$ -automaton  $Y$ .

Before we describe the influence weights generation process we set an axiom:

**Marginal influence axiom:** *The marginal influence of a  $q$ -automaton  $X$  on another  $q$ -automaton  $Y$  is the highest influence that  $X$  can exert on  $Y$  when combined with other influences.*

In other words, when  $q$ -automata  $X_1, \dots, X_n$  impart influences on a given one, say  $Y$ , the contribution of any  $X_i$  remains weaker than the influence that it individually exerts on  $Y$  assuming all the other influences inexistant. Therefore, the maximum influence weight equals 1 (or the 4-uple (1 1 1 1) as fuzzy number)<sup>1</sup>.

The algorithm for generating the fuzzy weights of the influences impinging on a given  $q$ -automaton consists in exploring the weight lattice associated with that  $q$ -automaton from the top (i.e. the node having the maximum weight) to the bottom of the lattice in a breadth-first manner:

- (1) Set  $w_{max} = (1 \ 1 \ 1 \ 1)$
- (2) For each node:
  - (2.1) Intersect the supports of its fuzzy values corresponding to its parents' values and the underlying fuzzy  $O(M)$  relations. Stop the generation process if the intersection is empty.
  - (2.2) Intersect the cores of its fuzzy values corresponding to its parents' values and the underlying fuzzy  $O(M)$  relations. Stop the generation process if the intersection is empty.

*/\* If one of the above intersections is empty, that means the weight lattice is (partially) inconsistent. \*/*

<sup>1</sup>We represent a fuzzy number as a 4-uple  $(a_1 \ a_2 \ a_3 \ a_4)$  where  $a_1 \leq a_2 \leq a_3 \leq a_4$ ; the intervals  $[a_1, a_4]$  and  $[a_2, a_3]$  are respectively the *support* and the *core* of the so designated fuzzy number.

- (2.3) If  $[a, b]$  and  $[c, d]$  are the respective non-empty intersections computed in steps 2.1 and 2.2, then the fuzzy weight corresponding to the node is  $(a \ c \ d \ b)$ .

Since the weight of an influence cannot be equal to zero, when the weight lattice is consistent, the algorithm yields  $n$  fuzzy weights  $w_1, w_2, \dots, w_n$  in  $]0, 1]$ .

**Example:** During a fed-batch fermentation process, the antifoam ( $AM$ ), the pressure in the fermentor ( $P$ ), the agitation speed ( $AG$ ) of the fermentation liquid, the oxygen inflow rate ( $O_2$ ) and the gaz inflow rate ( $Q_g$ ) influence the dissolved oxygen ( $DO$ ) in the fermentor. Let us denote the weight of  $X$  by  $W_X$ . The weight lattice associated with the dissolved oxygen is (fig.2): ( $W_{AG} \sim < W_{AM}$ ;  $W_{Q_g} - < W_{AM}$ ;  $W_{Q_g} \sim < W_{AG}$ ;  $W_P \sim < W_{Q_g}$ ;  $W_P - < W_{AG}$ ;  $W_{O_2} \sim < W_P$ ;  $W_{O_2} - < W_{AG}$ ). Applying the procedure above to that weight lattice where  $W_{AM}$  is the maximum weight, the following fuzzy weights are generated:  $W_{AM} = 1$ ,  $W_{AG} = (0.59 \ 0.77 \ 1 \ 1)$ ,  $W_{Q_g} = (0.35 \ 0.59 \ 0.59 \ 0.77)$ ,  $W_P = (0.21 \ 0.45 \ 0.59 \ 0.77)$  and  $W_{O_2} = (0.14 \ 0.35 \ 0.59 \ 0.77)$ .

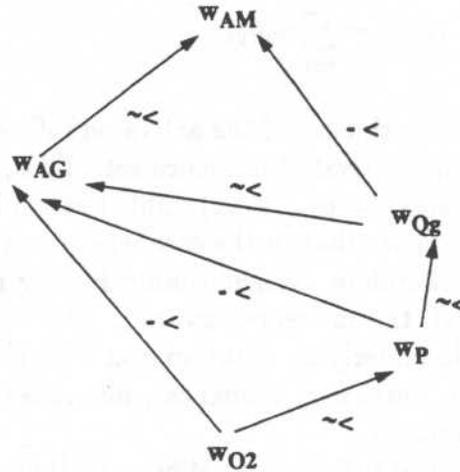


Fig.2: Weight lattice associated with the dissolved oxygen in a fed-batch fermentation process.

## 4 Simulation

We start this section with a definition that we shall use next. Let  $S = (a, b)$  be a real interval. We call *fuzzy truncature relative to S* the mapping denoted by  $T^S$  defined from the set of fuzzy numbers to the set of fuzzy numbers in  $S$  such that, for any fuzzy number  $r = (r_1 \ r_2 \ r_3 \ r_4)$ :  $T^S(r) = (r'_1 \ r'_2 \ r'_3 \ r'_4)$ , where for each  $i$ ,  $r'_i = \max(a, \min(r_i, b))$ , i.e.  $r'_i = a$  if  $r_i < a$ ,  $r'_i = r_i$  if  $r_i \in S$ , or  $r'_i = b$  if  $r_i > b$ .

### 4.1 Combining influences

Consider numeric q-automata  $X_1, X_2, \dots, X_n$  influencing another numeric q-automaton  $Y$  through influence-based relations. We denote the variation space of  $Y$  by  $\Delta Y$ , and the variation (change) of  $X_i$  on a relatively small time-interval  $\tau$  by  $\delta x_i$ , for each  $i$ . Let  $\delta y_i$  be the marginal influence of  $X_i$  on  $Y$  (i.e. the influence of  $X_i$  on  $Y$  assuming that there is no other influence on  $Y$ ) when the variation of  $X$  is  $\delta x_i$ . The problem of combining influences of  $X_1, X_2, \dots, X_n$  on  $Y$  is to describe the influence combining function of q-automaton  $Y$  which yields the weighted effects of the variations of  $X_1, X_2, \dots, X_n$  on  $Y$ .

The influence combining function of q-automaton  $Y$  is a mapping  $\odot : \Delta Y^n \rightarrow \Delta Y$ , which should meet the following conditions:

- (i) Consistency:  $\odot(0, \dots, 0, \delta y_i, 0, \dots, 0) = \delta y_i$

(ii) n-symmetry:

$$\odot(\delta y_1, \delta y_2, \dots, \delta y_i, \dots, \delta y_j, \dots, \delta y_n) = \odot(\delta y_1, \delta y_2, \dots, \delta y_j, \dots, \delta y_i, \dots, \delta y_n)$$

Consistency ensures no contradiction with regard to the concept of marginal influence; one of its consequences is  $\odot(0, 0, \dots, 0) = 0$ , that is, no change occurs in a q-automaton as long as no influence exerts on it. The n-symmetry condition ensures the unicity of the net influence underlying a set of marginal influences.

To compute the net influence, we must only consider activated influences. If  $I \subseteq \{1, 2, \dots, n\}$  is the subscript set of all the activated influences during the time-interval  $\tau$ , then for  $j \notin I$ ,  $\delta y_j = 0$ . In such a case, combining the effects of  $X_1, X_2, \dots, X_n$  on  $Y$  reduces to the combination of the effects of  $(X_i)_{i \in I}$  on  $Y$ . That suggests that we tune the weight of each activated influence to the overall set of activated influences while computing the net influence. The general form of the combining function we consider is:

$$\odot(\delta y_1, \delta y_2, \dots, \delta y_n) = \sum_{i \in I} w'_i \delta y_i \quad (1)$$

where  $I$  is the subscript set of the activated influences, and  $w'_i$  is the weight of the influence of  $X_i$  on  $Y$  tuned to the activated influence set. Thus, if all the influences intended to impinge on  $Y$  are activated, then  $w'_i = w_i$ . (Eq.1) fulfils the condition of n-symmetry. To meet the condition of consistency, we impose that in the case where only one influence is activated, the net influence equals that one. Therefore, weight tuning is only required when more than one influence are activated whereas all the influences are not. The  $w'_i$ 's depend on the  $w_i$ 's,  $i \in I$ , and on whether the process variable underlying q-automaton  $Y$  is an extensive variable or an intensive one. We call *extensive* (resp. *intensive*) influences, influences on a q-automaton assigned to an extensive (resp. intensive) variable.

**Case of extensive influences:** When the influences of  $(X_i)_{i \in I}$  on  $Y$  are extensive, we set, for each  $i \in I$ :

$$w'_i = T^U(w_i / \tilde{\max}_{j \in I} w_j) \quad (2)$$

where  $\tilde{\max}$  is the fuzzy maximum operation [5],  $U$  denotes the unit interval  $[0, 1]$ , and  $T^U$  the fuzzy truncature relative to  $U$ . The truncature operation guarantees that  $w'_i$  takes on values from  $]0, 1]$ .

**Proposition 4.1.1:** *If the influence having the maximum weight ( $w_{max} = (1 \ 1 \ 1 \ 1)$ ) in the weight lattice is activated, then for each  $i \in I$ ,  $w'_i = w_i$ .*

**Case of intensive influences:** That corresponds to averaging the influences of  $(X_i)_{i \in I}$ , hence we take for each  $i \in I$ :

$$w'_i = T^U(w_i / \sum_{j \in I} w_j), \quad (3)$$

and we impose the  $w'_i$ 's to be linked by the following equation since equation (1) should be a mean:

$$\sum_{i \in I} w'_i = 1 \quad (4)$$

Computing (1) under constraint (4) is termed as fuzzy interactive summation, which is thoroughly studied by Dubois and Prade [5].

Proposition 4.1.1 holds for the intensive case too. Furthermore, a property mimicking idempotency is met:

**Proposition 4.1.2:** *Let the influences on  $Y$  be intensive. If all the influence weights are identical, and so are the marginal influences, then the net influence on  $Y$  equals the common value of the marginal influences.*

## 4.2 Simulation Algorithm

The input data are the causal model - including initial conditions - and the evolution of the control variables of the process over time which may be data acquired on-line, recorded data, or data generated by mathematical functions. The output of the system is the behavior of each process variable which is displayed as the process runs. The simulation starts with the compilation of the causal model. The compilation consists in generating the fuzzy weights of influences, marginal influence tables according to the relative variation rates in the influence-based relations and partial description of these tables [2], tables containing influence delays and durations. The temporal unit of the simulation is that of a logical clock that is set according to the swiftness of the process.

The simulation is based on the propagation of influences through the causal network describing the interactions among the process q-automata. At each clock tick, the following steps are performed for each q-automaton starting from the control q-automata (i.e. q-automata associated with the control variables) in a breadth-first exploration of the causal network:

- (1) Update exogenous, and measured q-automata
  - /\* That consists in reading a data file or acquiring on-line data and computing the qualitative values (states) and variations for each exogenous, and measured q-automaton accordingly. \*/*
- (2) For each unmeasured q-automaton  $y$  do
  - (2.1) If (the q-automaton appears as the first argument of an information-based relation)
    - Then deduce its new state from the mapping describing that relation.
  - (2.2) Else
    - (2.2.1) Let  $\delta y(t)$  be the net influence at clock tick  $t$ . Compute the likeliest variation, that is, the element of the variation space which is the closest to  $\delta y(t)$  in the sense of the Hamming distance. Denote the likeliest variation by  $\delta y^*(t)$ .
      - /\* The likeliset variation is taken as the output influence of the q-automaton (i.e. the influence that the q-automaton exerts on other q-automata). \*/*
    - (2.2.2) Set  $y(t) = y^*(t-1) \dot{+} \delta y^*(t)$ , where  $y^*(t-1)$  is the most recent state of the q-automaton,  $\dot{+}$  the sum operator among intervals,  $\delta y^*(t)$  the likeliest variation at  $t$ .
      - /\* The quantity  $y(t)$  is an interval which may encompass several subintervals of the q-automaton's quality space. \*/*
- (3) Determine the new state of each q-automaton  $y$  by filtering the ranges of possible states  $y(t)$  (computed in step 2.2.2) out for consistency using the global (interval-based) constraints. The result of the filtering gives rise to a new state  $y^*(t)$  for each q-automaton (see hereafter for more details).

*Determining new states.* Since the ranges of possible states may contain several possible states, there is a need to refine them. This is done in two steps. First, the global constraints are used to restrict the extent of each interval  $y(t)$  (computed in step 2.2.2) in doing a tolerance propagation [8] on them (the new ranges may encompass more than one state too). Then, the new state is computed for each non-measured q-automaton as the likeliest state in the sense of the Hamming distance (similarly to the computation of likeliest variations). However the lower and the upper

states may be optionally calculated. The above mentioned three states are computed for their relevancy. Indeed, the upper (resp. lower) state corresponds to the most germane overestimation (resp. underestimation) of the state of the q-automaton, the likeliest state is interpreted as its most probable state. The simulation process retains (displays and records) all the three states but the likeliest state is taken as the state for the current time-point.

## 5 Example application to fed-batch fermentation

Cultures in the biotechnological industry are based on the degradation of a substrate ( $S$ ) by a population of micro-organisms, the biomass ( $X$ ), into metabolites. The type of fermentation in biomass production depends on the way that fresh nutrients are fed into the fermentor. Fed-batch fermentation is characterized by the fact that it starts with an initial volume of nutrients; then the action variables (antifoam ( $AM$ ), gas inflow rate ( $Q_g$ ), oxygen inflow rate ( $O_2$ ), agitation ( $AG$ ), pressure ( $P$ ), etc...) are acted upon, and additional nutrients are brought during the fermentation process if need be. A fermentation process aims to increase the concentration rate of biomass so as to obtain the maximum concentration of product through the use of a suitable substrate and oxygen feeding.

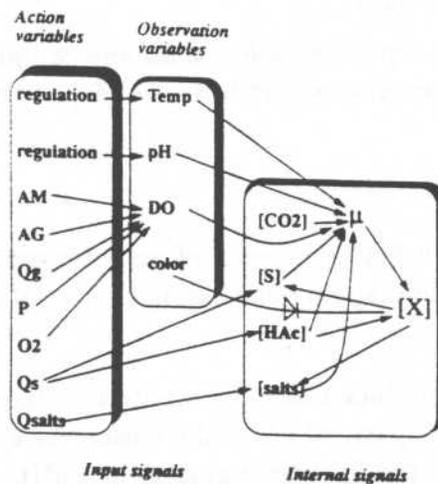


Fig.3 Causal network of a fed-batch fermentation process.

- AM : antifoam
- AG : agitation
- $Q_g$  : gas inflow rate
- $P$  : pressure in the fermentor
- $O_2$  : oxygen inflow rate
- $Q_s$  : substrate inflow rate
- $Q_{salts}$  : mineral salts inflow rate
- Temp : temperature of the liquid in the fermentor
- pH : pH of the liquid in the fermentor
- DO : dissolved oxygen
- color : color of the liquid in the fermentor
- $[CO_2]$  : concentration rate of  $CO_2$
- $[S]$  : substrate concentration rate
- $[HAc]$  : acetic acid concentration rate
- $[salts]$  : mineral salts concentration rate
- $\mu$  : biomass specific growth rate
- $[X]$  : biomass concentration rate

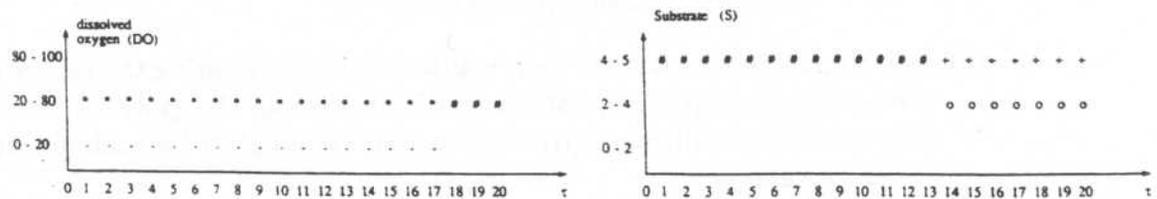


Fig.4. Simulation results. + = upper state; - = lower state; \* = upper and likeliest state; o = lower and likeliest state; \$ = likeliest state; # = upper, lower and likeliest state.

Fig.3 depicts the network of causal influences among the relevant variables of the process. In our process plant, dissolved oxygen (DO) is the witness variable on which commonsense interpretations

of the process behavior rely as studied by Steyer [14]. To show what kind of information we can get from the simulation based on the method presented above, the behaviors of dissolved oxygen and substrate resulting from the simulation of the causal network are presented in fig.4, for  $\tau = 0$  to 20, i.e during 60 seconds. The quality spaces of  $DO$  and  $S$  are respectively  $\{[0, 20[; [20, 80[; [80, 100]\}$  and  $\{[0, 2[; [2, 4[; [4, 5]\}$  as provided by the process experts; interval  $[20, 80[$  is the nominal range of  $DO$ . The initial conditions for these variables have been taken equal to 40 and 4.5 respectively, and we assume that no more substrate is fed then. The temporal unit considered is three seconds.

Fig.4 shows that the likeliest state of  $DO$  is normal (falls into the nominal range) till  $\tau = 20$ , but the lower state remains in interval  $[0, 20[$  till  $\tau = 17$  then it goes up to interval  $[20, 80[$ . The increase of the lower state is interpreted as a possible increase of the dissolved oxygen although its actual value remains qualitatively unchanged. That increase in  $DO$  can be explained by the fact that the bacteria consume less oxygen than fed into the fermentor because of the metabolites slowness at the beginning of the fermentation process. In fact, ten to fifteen minutes after the start of the process, the dissolved oxygen begins to decrease. The lower state, likeliest and upper state of substrate are the interval  $[4, 5]$  from  $\tau = 0$  to  $\tau = 13$ , then the likeliest and lower states decrease to interval  $[2, 4[$ . That means the substrate concentration rate decreases, which is quite normal, since no more substrate is fed into the fermentor whilst the bacteria grow and consume the initial substrate.

The simulation of the causal network allows to continuously estimate the state of non-sensored variables (such as substrate in our process plant) during the proces life-time. It is also a means to detect possible misbehaviors beforehand so as corrective actions can be taken to keep the process in suitable conditions.

## 6 Discussion and Perspectives

This paper presents a causal simulation method for incompletely known dynamic systems in process engineering. The causal model of a process is represented as both a causal network of interacting elementary dynamic systems, called qualitative automata, influencing one another, and a set of qualitative constraints linking possibly several of such automata. Associated with each influence is a weight which expresses its sensitivity. A procedure is presented which allows us to generate fuzzy weights from the relative order of magnitude relations between them. Formulae preserving non-linearities and fulfilling some relevant requirements are provided to compute net influences on extensive variables as well as on intensive ones. Finally an algorithm is given for simulating the causal model.

The advantages of the proposed approach over existing ones are : 1) the consistency checking of relative weights provided by experts and the generation of fuzzy weights from their relative description, 2) the computation of net influences takes into account non-linearities and the fact that the influences can be extensive or intensive, 3) the simulation algorithm has been devised so as it can be used for real-time applications in process engineering, because instead of generating all the possible behaviors - which may make it burst - it focuses on the relevant behaviors (i.e. upper, lower and likeliest states). However, the patent shortcomings of the approach are that 1) it does not account for numerical equations which may be accurately known and useful for some processes, 2) it relies on the causal network provided by an expert and has no means to perform causal analysis of the process at hand. The former drawback can be solved by performing a causal analysis of equations as studied by Rose and Kramer [12], and then using the results of that analysis to build the causal chart, the latter is a major challenge in Qualitative Physics.

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