Qualitative modeling techniques for process control and diagnosis*

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ABSTRACT: Qualitative reasoning is an alternative to mathematical modeling and can be used to reason about unforeseen situations that are not encoded in the knowledge base.

KEYWORDS: Bleaching, chemical reactions, chemical treatment, chlorination, diagnosis, halogenation, models, process control, simulation.

Qualitative reasoning (QR) is a subarea of artificial intelligence (AI) that reasons about the physical world using qualitative representations. Qualitative models capture the underlying mechanisms of the physical system and overcome the brittleness found in heuristics-based expert systems that cannot reason about unknown or unanticipated problems. In addition, QR does not require a complete model of the system in order to reason. It can work with partial knowledge and information, thus overcoming some of the difficulties of mathematical modeling.

QR has received considerable attention from the AI community in recent years and a variety of approaches have been developed *(1, 2)*. Some of these are application specific while others are more general. The general approaches differ mostly in the primitives used to describe the physical system and they include:

1. A component-centered approach *(3, 4)* wherein the system is modeled as a device made up of components and the connections between them. It derives the behavior of this device by using the connections (or confluences) to constrain the possible behaviors generated.
2. A process-centered approach *(5)* that models the system in terms of objects and processes, a process being something that causes changes to objects over time. A process is activated when its conditions are met and the necessary objects are present. It uses the set of active processes to derive the qualitative constraint model used to generate the possible behaviors of the system.
3. A constraint-based approach *(6, 7)* that models the system as a set of qualitative constraint equations. Unlike the previous two approaches where the modeler describes the system in terms of abstractions (such as processes and components), with the constraint models automatically generated from these, this approach does not attempt the translation from the physical world to the qualitative model (i.e., the modeler is required to manually construct the qualitative constraint model).

From the constraint model, generated by applying one of these three approaches, qualitative simulation predicts the possible behaviors of the system.

In this paper, we focus on the constraint-based approach to qualitative reasoning using an algorithm called qualitative simulations (QSIM) *(7)*. In the next section, we explain the basic concepts of QSIM using a simplified pulp bleaching example. Further on, we discuss how this can be used to do fault diagnosis.

Basic QSIM

QSIM is an algorithm developed by Benjamin Kuipers to do qualitative simulation given a qualitative system structure description and an initial state. It provides a representation language where the system structure is described using qualitative differential equations (QDEs). QDEs represent abstractions of ordinary differential equations or incomplete knowledge of the system. QSIM also provides the qualitative mathematics required to simulate the behavior of the system from the QDEs. It predicts possible system behaviors and produces a graph showing the future system states.

To illustrate the concepts of QSIM, we use a simplified model of the chlorination stage of the bleaching process.

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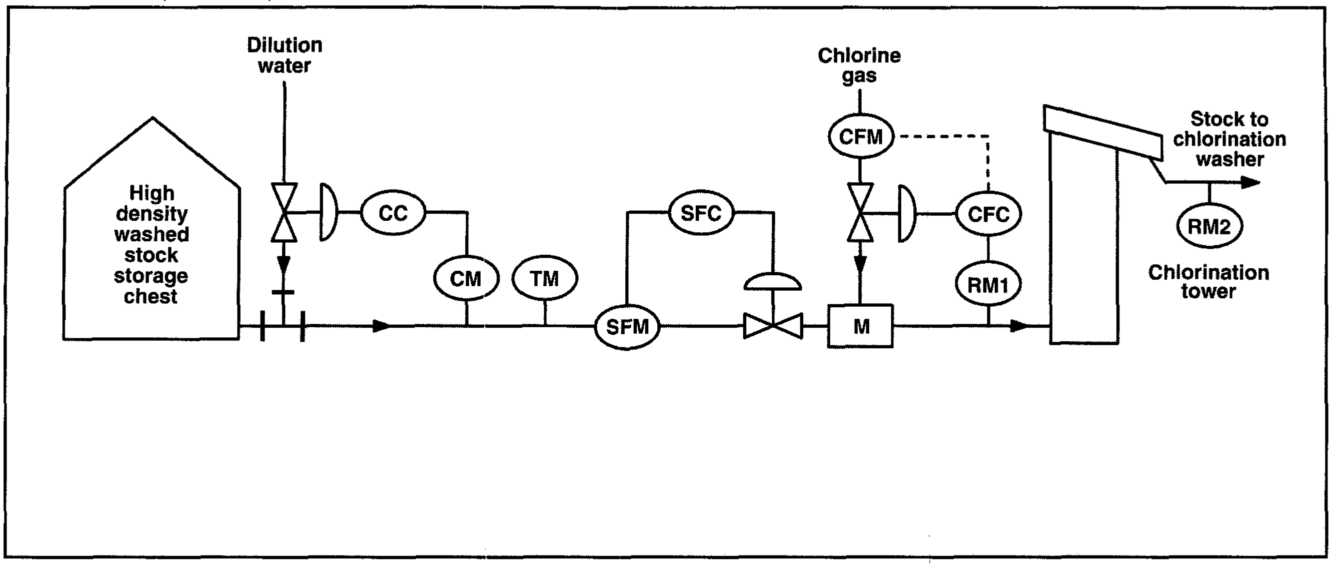
1. Chlorination stage of pulp bleaching process. Shown are: consistency meter (CM), consistency controller (CC), temperature measurement: (TM), stock flow meter (SFM), stock flow controller (SFC), chlorine flow meter (CFM), chlorine flow controller (CFC), mixer (M), and chlorine residual meters (RM1, RM2)



Chlorination stage of pulp bleaching

Figure 1 and the corresponding block diagram of **Fig. 2** represent an example of the chlorination stage of a pulp bleaching process. The injection water used with the chlorine gas is not shown explicitly. The chlorine valve is controlled such that the input residual R_i, measured as a percentage of dry chlorine on dry pulp, will be regulated to the input residual setpoint R_{i*}.

Let the input residual setpoint R_{i*} be determined such that the output residual R_o will be a small value R_{on} under specified nominal values of stock flow F_{sn}, temperature T_n, and consistency C_n assuming a normal flow distribution in the chlorination tower as characterized by the nominal retention time T_m. The values R_{on}, F_{sn}, T_n, C_n, and T_m are nominal values of the corresponding variables R_o, F_s, T, C, and T_r. We assume also that the setpoint R_{i*} is not adjusted for variations in these variables. Furthermore, although R_{i*} would usually be adjusted as a function of the kappa number of the unbleached pulp, it is sufficient for our purposes to consider the constant kappa number case.

For a chlorination tower of height H (m) and effective cross-sectional area A_e (m^2) from a flow distribution viewpoint), the retention time T_r (s) is given by Eq. 1:

$$T_r = HA_e/F_s \tag{1}$$

where

F_s = stock flow, m^3/s.

When channeling occurs in the tower, the flow distribution is impaired such that A_e is decreased.

Defining the kappa factor as the ratio of percentage chlorine gas on dry pulp to the kappa number of unbleached pulp, experience shows that the kappa factor decreases approximately linearly as a function of log T_r. For kappa factor values in the typical range [0.19, 0.26], the corresponding range of time to consume all the chlorine is 9–65 min, or 540–3900 s. Therefore, the following steady state model is proposed.

$$R_o = R_i[1 - F(C,T)G(T_r)],\ FG \le 1 \quad \text{(2A)}$$

$$= 0,\ FG > 1 \quad \text{(2B)}$$

where

$$G = \log(1 + T_r^2)^{1/2} \tag{3}$$

and F is a positive function of consistency C and stock temperature T with the property that it increases if C and/or T increases, reflecting the fact that R_i decreases with increases in C or T (or both).

The value of F under nominal operating conditions can be determined by substituting nominal values into Eq. 2A and solving for F:

$$F(C_n,T_n) = (R_{in} - R_{on})/[R_{in}G(T_m)] \tag{4}$$

We could also attempt to derive an analytical expression for $F(C,T)$, as was done for $G(T_r)$ in an effort to obtain an entirely quantitative model, but this is not necessary for qualitative modeling.

Equation 3 yields the following approximations:

$$G \sim \log T_r,\ T > 1 \quad \text{(5A)}$$

$$= 0.151,\ T_r = 1 \quad \text{(5B)}$$

$$\sim 0,\ T_r <= 1 \quad \text{(5C)}$$

The accuracy of the approximations increases as a function of the strength of the T_r inequalities. Applying Eq. 5 to Eq. 2A, we obtain:

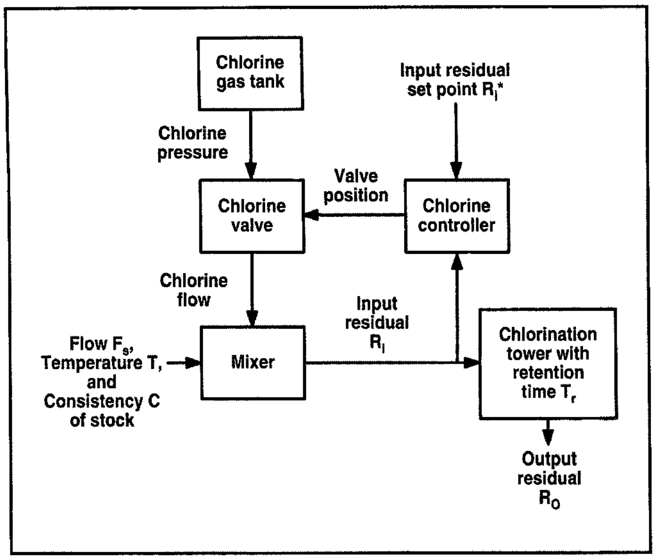
$$R_o \quad R_i[1 - F(C,T)\log T_r],\ T_r > 1 \quad \text{(6A)}$$

$$= R_i[1 - 0.151]F(C,T)],\ T_r = 1 \quad \text{(6B)}$$

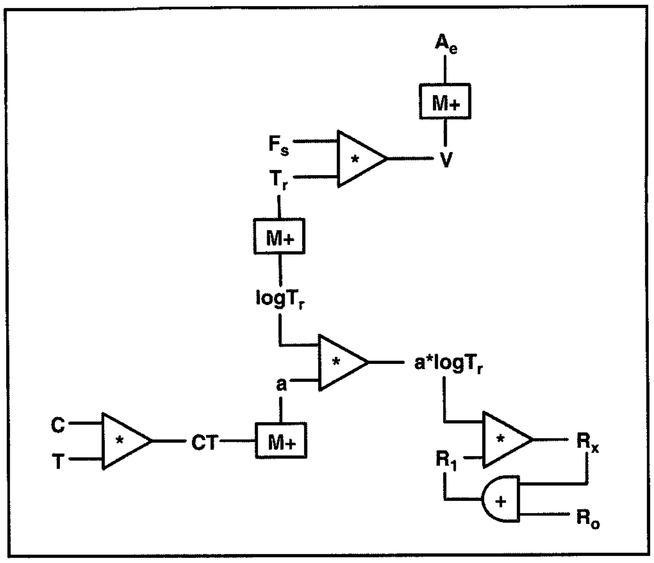
$$\sim R_i,\ T_r < 1 \quad \text{(6C)}$$

For typical values of T_r greater than 540 s (9 min), Eq. 2 is seen to be an excellent approximation reflecting the variation of kappa factor (hence chlorine, given a constant kappa number) as a linear function of log T_r.

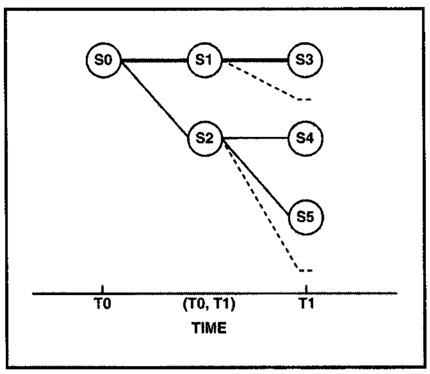
2. Chlorination control block diagram



3. Constraint network for the chlorination example



4. Tree of possible behaviors generated by QSIM. *T0* and *T1* are system-distinguished time points. *S0*, *S1*...*S5* are system states defined by a qualitative state for each parameter. The path from *S0* to *S3* shown in bold represents one possible behavior



Defining the system structure

The system structure is described to QSIM in terms of a set of parameters and a set of qualitative constraint equations. The parameters represent the state of the system and the equations define relationships between the parameters to describe the structure of the system.

QSIM assumes that each parameter is a real-valued continuously differentiable function of time. Each has an ordered set of landmark values which are numeric or symbolic values of the function at its critical points or which specify the upper and lower range limits of the operating region of the parameter. For example, the input residual R_i, is defined to have the initial set of landmark values of (0, R_{i*}, infinity). This limits R_i to values between 0 and positive infinity, and it defines R_{i*} as its setpoint, an important value for R_i, which lies in this range.

Instants of time when something interesting happens to the value of a parameter are called distinguished time points (e.g., when a parameter passes by a landmark value). Time is viewed by QSIM as a totally ordered set of symbolic distinguished time points. The current time may then be either equal to a distinguished time point, e.g., *T0*, or to an open interval between two adjacent distinguished time points, e.g., *T0.T1*.

The *qualitative state* of a parameter p at a time t, QS (p,t), is a pair composed of a qualitative magnitude and a direction of change. The qualitative magnitude is the value of the parameter in terms of its ordinal relations with landmark values. This value may either be equal to a landmark value, e.g., R_{i*}, or to an open interval between two adjacent landmark values, e.g., 0,R_{i*}. The direction of change of the parameter at time t can be increasing, steady, or decreasing. Therefore, QS($R_i t_j$) may be equal to (R_i, steady). The qualitative behavior of the parameter is a sequence of its qualitative states.

There are three types of qualitative constraints in QSIM *(6)*.

1. Arithmetic constraints that constrain the values of the parameters to have the indicated relationship at each point in time (e.g., ADD, MULT, MINUS)
2. Derivatives that specify the rate of change of a parameter
3. Functional relationships which are used when there is need to state that one parameter is a function of another without specifying this function completely [e.g., $Y = M+ (X)$ to represent the knowledge that Y is a strictly increasing function of X (and M- for decreasing)].

From the incomplete mathematical model of the chlorination stage of the bleaching process discussed earlier, a set of corresponding (but weaker) QDEs are defined. For example, the linear function between the effective cross-sectional area of the chlorination tower and its volume ($V = A_e H$) is mapped to the M+ constraint between A_e and V. This mapping makes the model applicable to a larger set of systems. The qualitative model is graphically represented in a constraint network shown in **Fig. 3.**

In addition to the structural description of the system, QSIM also requires an initial state from which to start the prediction. This is a partial or complete specification of the initial qualitative states of the system parameters. QSIM performs constraint propagation to complete the initial state definition. It then applies rules to determine the valid transitions for each parameter. It uses the qualitative constraints and some global filters to reduce the number of possible state transitions. It may be that in the end there are multiple possible transitions from the current state. QSIM then produces a branching tree of possible behaviors. Although Kuipers proves that this algorithm will produce all possible real behaviors, it may also produce spurious behaviors *(7)*.

Results

The output of QSIM is one or more qualitative behavior descriptions for the system, graphically represented as a branching tree. (See **Fig. 4.**) A node in the tree represents a system state. A path through the tree from the root node or initial state to a leaf node or final state represents one possible system behavior. Each behavior consists of: (a) a sequence of system-distinguished time points (the union of the distinguished time points of the individual functions or parameters), (b) an ordered set of landmark values for each parameter, and (c) a qualitative state for each parameter at each system-distinguished time point and the interval between adjacent time points.

Given that the chlorination tower is perturbed from steady state by a decrease in the effective cross-sectional area of the tower A_e, QSIM predicts many possible next states. One such state has the input residual R_i constant at its setpoint and the stock flow F_s, temperature T, and consistency C at their nominal values. **Figures 5A and 5C** show two behaviors predicted from this next state. (An example of another possible next state keeps the temperature, stock flow, and consistency at their nominal values, but the input residual deviates from its setpoint. **Figure 6** shows one behavior predicted from this next state.) The system-distinguished time points are shown at the bottom of each graph (with NORMAL showing steady state). The landmarks for the parameter are shown (vertically) at the right of the graph for the parameter. In Fig. 5A, the graph for the cross-sectional area shows that this parameter starts off at time *T0* having a qualitative magnitude of AE^* (read as A_{e*}) and a direction-of-change of decreasing. It reaches a new landmark value *AE*-0 at time *T1* and holds at this value. This change has affected the retention time T_r and the output residual R_r. The retention time also decreases down to a new landmark value, *TR*-0, whereas the output residual increases to a new landmark value, *RO*-0, which is greater than its nominal value, *RON*. Figure 5B is another possible behavior predicted by QSIM. It is different from that shown in Fig. 5A in that the effective cross-sectional area decreases all the way to zero.

Limitations of QSIM

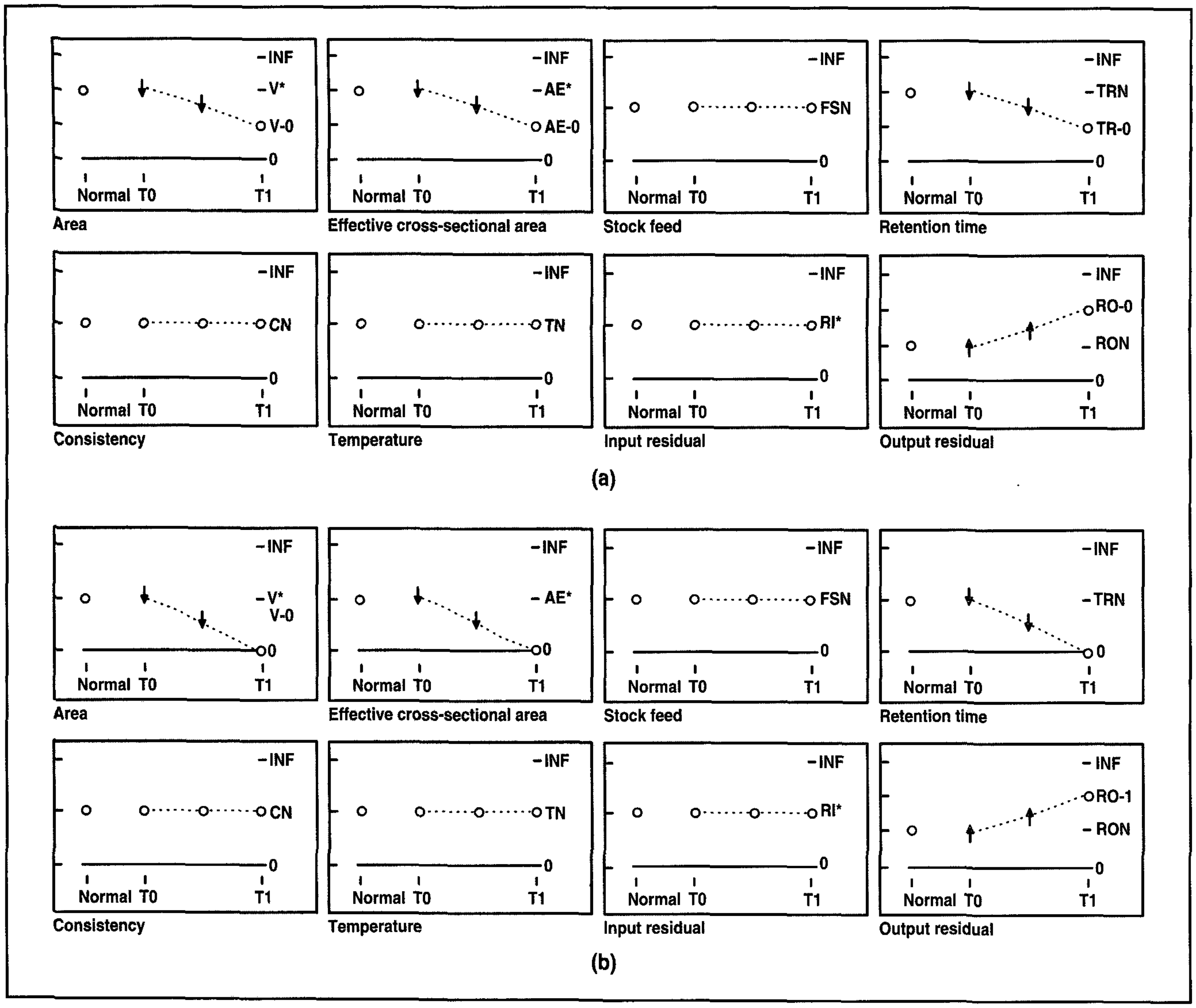
QSIM has been used to simulate different systems such as the water and sodium balance mechanisms in medical physiology *(8)*, chemical reaction systems *(9)*, simple tank systems (e.g., cascaded tanks and coupled tanks), etc. Several limitations of this technique have been pointed out *(10)*.

Firstly, the tree of possible behaviors produced by QSIM may be intractable and may represent spurious behaviors. (Fig. 5B, discussed earlier, provides an example of spurious behavior. A_e goes to zero and this, of course, is not practical). One cause is the ambiguity found in the qualitative mathematics. The results of calculations are not always unique. For example, in the qualitative model of the chlorination tower, the volume is equal to the product of the retention time and the stock flow ($V = T_l F_s$). The chain rule of calculus states that the derivative $V' = T_r' F_s + T_r F_s'$. Using (a) the derivative of V to determine its direction of change, i.e., if $V' > 0$ it is increasing, if $V' = 0$ it is steady, and if $V' < 0$ it is decreasing, (b) the knowledge that all three parameters are always positive or zero (from their landmark value definitions), and (c) the observations that T_r is increasing (i.e., $T_r' > 0$) and F_s is decreasing (i.e., $F_s' < 0$); qualitative mathematics will predict that the direction of change for V may be either increasing, steady, or decreasing (i.e., V has at least three possible qualitative values because of the three directions of change). This is because the qualitative result of multiplying T_r' and F_s (or T_r and F_s') is not known except that it is positive (or negative) and then adding a positive number to a negative number yields a value which is either > 0, $= 0$, or < 0. A second cause is that the qualitative model is an abstraction of the mathematical model and may thus apply to a bigger class of systems. Therefore, some behaviors predicted by QSIM may be spurious with respect to the systems modeled by the algebraic and ordinary differential equations, but may not be spurious with respect to other systems that satisfy the qualitative constraints.

To eliminate irrelevant or spurious behaviors, QSIM has been extended:

1. To incorporate a higher order derivative constraint *(11)* called the curvature constraint that eliminates one source of spurious predictions, that is, the lack of derivative information
2. To change the level of descriptions *(11)* so that large sets of behaviors whose distinctions are real, but not important, are grouped together
3. To incorporate incomplete quantitative information *(12)* that provides bounds for the landmark values, distinguished time points, and functional relationships (M+ and M-) between parameters. This eliminates behaviors that do not satisfy this quantitative knowledge.
   We have implemented an alternative method to *(12)* to incorporate quantitative information to QSIM. Our extension uses the Quantity Lattice approach of Simmons *(13)* to determine the relationships between quantities and to constrain the values of the parameters of an

5. Two possible behaviors of the bleaching example where the effective cross-sectional area is made to decrease and the input residual remains at its setpoint value, R_i. (a) The cross-sectional area, retention time, and output residual each reach another landmark value and hold there at time $T1$. (b) The cross-sectional area and retention time go down to zero and the output residual reaches a new landmark value



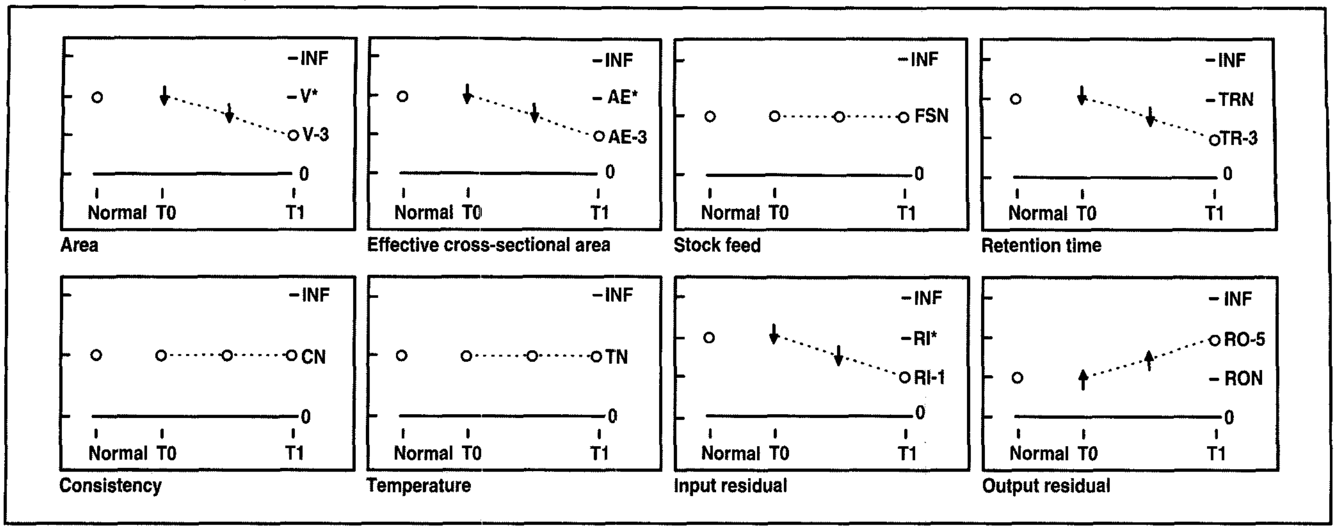
arithmetic expression. In addition to interval arithmetic, it uses relational arithmetic and constant elimination arithmetic to constrain the values of the parameters.

4. To incorporate other constraints such as the non-intersection of phase space trajectory constraint *(14)*.

Secondly, QSIM does not provide a formalism for creating an initial model. The modeler is required to manually derive the QDEs from a partial mathematical model and from incomplete knowledge of the system. To facilitate the model-building task, a model builder called QPC *(15)* has been developed based on the process-centered approach of the Qualitative Process Theory *(5)*. QPC assembles a QDE model and an initial state from the view-process structure and scenario descriptions. It then uses QSIM to do qualitative simulation.

Thirdly, QSIM and all other methods of qualitative simulation perform limit analysis. When several parameters are changing and possibly moving to some limit, the constraints among them are used to determine which of these actually reach their limits. This determines which qualitative states follow. For small systems, the constraints may be sufficient to keep the number of limit hypotheses to a reasonable size. For example, if you have two parameters a and b such that $QS(a,t_i) = (a_1, \text{steady})$ and $QS(b,t_i) = (b_1, \text{steady})$, then $QS[a,(t_i,t_{i+1})]$ and $QS[b,(t_i,t_{i+1})]$ each have three possible values. These are (a_1, steady), $[(a_1,a_2), \text{inc}]$, or $[(a_0,a_1), \text{dec}]$ and (b_1, steady), $[(b_1,b_2), \text{inc}]$, or $[(b_0,b_1), \text{dec}]$, respectively. $QS[a,(t_i,t_{i+1})]$ and $QS[b,(t_i,t_{i+1})]$ may then be combined in nine possible ways. However, given the constraint $a + b = c$ and the information that c is increasing at time (t_i,t_{i+1}), four of these possibilities are removed, e.g., (a_1, steady)

6. A possible behavior of the bleaching example where the effective cross-sectional area is made to decrease and the input residual deviates from its setpoint value, R_i.



and (b_1, steady) will contradict the information that c is increasing. For more complex systems, the number of changing variables that reach limits may be too large. Kuipers suggests a method of hierarchically decomposing these complex systems into less complex tractable subsystems using time-scale abstraction *(8)*. This method decomposes the complex system into equilibrium mechanisms that operate at varying time-scales; a faster mechanism is viewed by a slower one as being instantaneous, and a slower one is viewed by a faster one as being constant.

Finally, the qualitative models built are limited to those that can be described using the qualitative constraints supported by QSIM (e.g. arithmetic, derivative, and functional relationships). QSIM will have to be extended to support other types of constraints required for other domains. For example, Bridgeland *(16)* has had to extend QSIM to support the modeling of financial applications.

QR and fault diagnosis

Many systems that perform fault diagnosis represent the necessary knowledge as sets of rules that encode cause-and-effect relationships, e.g., Mycin *(17)*, or as diagnostic trees that are built from examples of known failures. Rule sets can be difficult to create, modify, and verify. Diagnostic trees depend on the completeness of the training set used to build them and do not cope well with faults that have not been encountered previously. Both methods are difficult to use in process environments where the systems are dynamic and where not all parameters of the system are measured (or measurable) or accessible. Recent work in qualitative reasoning has led to approaches that, because of a deeper representation of the process, are more effective for diagnosis (and control) of dynamic processes. We describe one such approach developed by Dvorak and Kuipers *(18)* that is used with QSIM and is called MIMIC.

Initially, a model of the physical system is built as described earlier in terms of QDEs. Some of these QDEs are further developed to specify system behavior that is based on normal and faulty operation of the components that they model. From this enhanced description of the physical system, a model building program generates the normal no-fault model, single-fault models, and possibly selected multiple-fault models. QSIM is then used to simulate each of the generated models from all possible initial states to give what is called the *total envisionment* for each model. From the states of the total envisionment, it is possible to produce a training set using the magnitude and direction of change of the *observable* parameters in the model. Each example in the training set is associated with the fault-combination of the model from which it was generated. An inductive process similar to the ID3 algorithm of Quinlan *(19)* is then applied to form a diagnostic decision tree. (MIMIC actually extends this technique to include other relevant information that helps to rank faults. This extra information includes *a priori* probability of faults and historical probabilities of behaviors.) Note that since the examples are generated from models of faulty and normal systems, and assuming that the models are accurate, a more complete set of examples is expected to be synthesized than might be collected from historical observations and prior diagnosis alone.

With the diagnostic tree in place and the qualitative models developed, we can monitor the process and diagnose faulty operation. MIMIC follows a hypothesize-and-match cycle with four basic steps.

1. Generate Hypotheses. In this step, observations of the process are interpreted [see Forbus *(20)*] for an interesting treatment of the interpretation of data collected from physical systems) and used in conjunction with the diagnostic tree described above to generate ranked hypotheses of faults.

2. Build Models. QSIM fault models based on the hypothesized faults of Step 1 are instantiated and added to the list of models being *tracked.* Only the n most promising models are actually tracked at one time.

3. Simulate Models. Each new model from Step 2 is initialized from the current observations and simulated as observations change to predict possible future states.

4. Match Observations to Tracked Models. A similarity function is then used to compare the observed values with the simulated model values and only models that meet threshold criteria are retained in the list of models being tracked.

As the cycle repeats itself, there may be one or more models being tracked. Over time, hypotheses will be rejected or confirmed, and the list should converge on a single candidate or a minimal list of most promising possible faults. In this method, qualitative modeling and simulation work together with the diagnostic tree to perform diagnosis in dynamic process applications. Consider the chlorination stage example again. Assuming that the necessary work has been done to generate all of the required fault models as well as the no-fault model and subsequently the diagnostic tree has been generated, the following sequence of events might occur. Initially the system is operating normally, and the no-fault model is being tracked. At some point, an increase in the output residual R_0 is observed. This is sufficient to cause the diagnostic tree to generate a hypothesis that the effective cross-sectional area A_e of the tank is decreasing. The model for this fault is placed on the list of tracked faults (the no-fault model is removed). If subsequent observations continue to support this fault model, then the fault is confirmed and corrective actions are taken. Other factors such as temperature T and stock flow F_s could influence the value of R_0 to make an increase, but since none of these measurable parameters have changed, the only possibility determined by the diagnostic tree is that A_e was decreasing.

This diagnostic method can be used with process systems that have few observable parameters. The diagnostic tree is used to limit the number of models that need to be tracked and the qualitative models and simulation allow the tracking of the hypotheses dynamically. The method has limitations and requires practical experience to improve and expand it. It assumes that faults will occur one-at-a-time with respect to the sampling rate, and conditions can occur that violate this constraint. Also the handling of multiple faults needs further study.

Conclusion

QR provides an alternative to mathematical modeling for domains where only partial knowledge and information are available. It also complements heuristics-based expert systems by providing a representation of the underlying mechanisms of the physical system. This can be used to reason about unforeseen situations that are not encoded in the knowledge base.

In this paper, we give an introduction to QR and how it can be applied to fault diagnosis. Our preliminary investigation of this technique leads us to believe that this is a promising approach. Much research has been done in QR, especially in improving the qualitative mathematics underlying this. It has been tested using laboratory systems, and some limitations have been identified and solved. Although QR is now being tested in practical systems *(21)*, it is still very much a research area. In addition, much work remains to be done to incorporate this technique into a comprehensive expert system that performs a task such as fault diagnosis, plant monitoring and control, or operator training.

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