JELENKA B. SAVKOVIĆ–STEVANOVIĆ

Department of Chemical Engineering, Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

SCIENTIFIC PAPER

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THE CHEMICAL PLANT MANAGEMENT QUALITATIVE SUPPORT SYSTEM

The aim of this paper was to capture the benefits of common sense qualitative reasoning about process phenomena as displayed in the human behaviour mental model. The control features of qualitative modeling and simulation were qualitative variable description and logic rules for manipulating variable values between systematic states. The additional measure of qualitative information value was introduced. This study is the first report in the literature showing the measure of qualitative information value. Qualitative simulation was applied to the fault diagnosis of a chemical system. The obtained results illustrated the goodness of the estimation of system behaviour during an abnormal situation. The developed qualitative simulator for fault doagnosis generates original scenarios and can serve as a useful aid to a system operator.

Qualitative reasoning is a relatively new field of study stemming from fundamental research in qualitative physics, qualitative process theory, common sense knowledge and naïve physics.

In qualitative process description, each phenomenon is described by preconditions, constraints and influences [1–4]. The preconditions must be satisfied for the phenomenon to become active. When the preconditions are met, constraints are qualitative equations describing parameters associated with the phenomenon, and influences are the driving forces of a phenomenon and describe how changes occur as a result of the phenomenon being active [5,6].

The qualitative states of all the variables in a plant or device define the state of the system or device [1,7–11]. For example, to activate the phenomenon of heat flow, there must be two objects (a source and a destination) with the temperature of the source greater than that of the destination. Also, there must be a common, non–insulated wall between them.

The qualitative process engine–QPE automatically generates process centred qualitative simulation models [12–15], which consist of a network of causal constraints. In QPE, each phenomenon (i.e. chemical reaction, liquid flow, heating, cooling etc.) is described by preconditions, constraints and influences [2,3,9]. Synthetic fiber production was chosen as a case study in this paper. A qualitative simulation environment was developed and information processing was performed for a management support system.

Author address: J.B. Savković–Stevanović, Department of Chemical Engineering, Faculty of Technology and Metallurgy, The University of Belgrade, Karnegijeva 4, 11000 Belgrade, Serbia and Montenegro
E–mail:savkovic@elab.tmf.bg.ac.yu
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A QUALITATIVE SIMULATION ENVIRONMENT

A qualitative simulation environment provides a means for utilizing qualitative reasoning within a computerized environment to simulate the behaviour of the system. The system can currently perform fault diagnosis in a plant consisting of pumps, valves, tanks, reactors and streams. No limitation is placed on the number of equipment units or streams, since it is a simple matter to create a new frame and working memory element. Initial research starts by the phase of the development of a conceptual framework, which will facilitate the modular specification of the models, and continuous with a second phase, the development of a logic framework, which will permit object using attributes and simulation techniques to be linked into executable models (Figure 1). The first framework is a modular view of a processing system as a collection of entities and interactions. The active flow operates by the use of rules

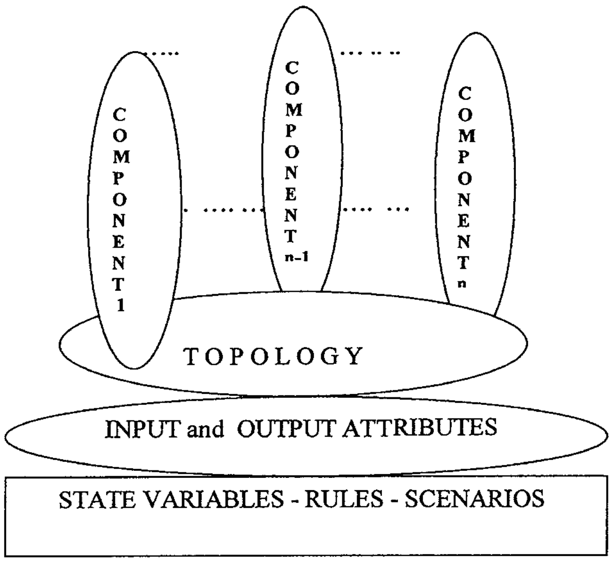

Figure 1. Qualitative modeling

in the knowledge base. The passive flow is the interface between the simulator and a user establishing attribute sets, the initial state and symptoms.

The production of synthetic fibers was chosen as a case study. Also, the system can diagnose for causes of faults associated with state variable pressures, flow rates and temperatures. The qualitative variables are described in three discrete values low, medium and high. Equipment states are also described in qualitative terms such as closed, open, failed, blocked and leak. The following faults are considered: blockage, leakage, malfunction or misoperation. The study of fault detection and diagnostics is concerned with designing a system that can assist a human operator in detecting and diagnosing equipment faults in order to present the accident state which describes the variable relative location to landmarks (boiling point or maximum pressure) and the sign of their first derivatives. It can be used to identify what problems in the initial scenarios cause subsequent symptoms in the working model.

QUALITATIVE INFORMATION PROCESSING

In the qualitative simulation phase, the model set forth in the previous system definition phase is simulated. Each component, represented by an individual set of causal rules, is executed in sequence. After every component the resultant symptomatic state is compared with the prior symptomatic state. If the states are identical, then steady state is achieved and the simulation is halted. If steady state is not achieved then the simulation continues until steady state is eventually achieved or an upper allowable value. This procedure is repeated for each scenario specified in the system definition phase of the architecture. The algorithm for executing a simulation model is shown in Figure 2.

With the completion of the qualitative simulation runs, a resultant symptom/scenario matrix is formed. The symptom scenario matrix represents the steady state nature of each scenario by displaying the final values of each symptom. One of the powerful features of qualitative simulation is that it readily allows for different sets of state variable values to lead to common scenario simulation results. In the symptom decomposition phase, the relational symptom/scenario matrix is decomposed by using a projection operation that delineates which scenarios were found to have the same symptom values in their final state.

In the final optimal sequencing phase the symptoms are ordered by relative information value or use within a decision tree. The order is determined by the relative number of scenarios each symptom delineates, the probability of each scenario occurring, and the expense associated with the testing for each symptom. This optimal sequence is not only dependent upon the time it takes to observe each symptom, but

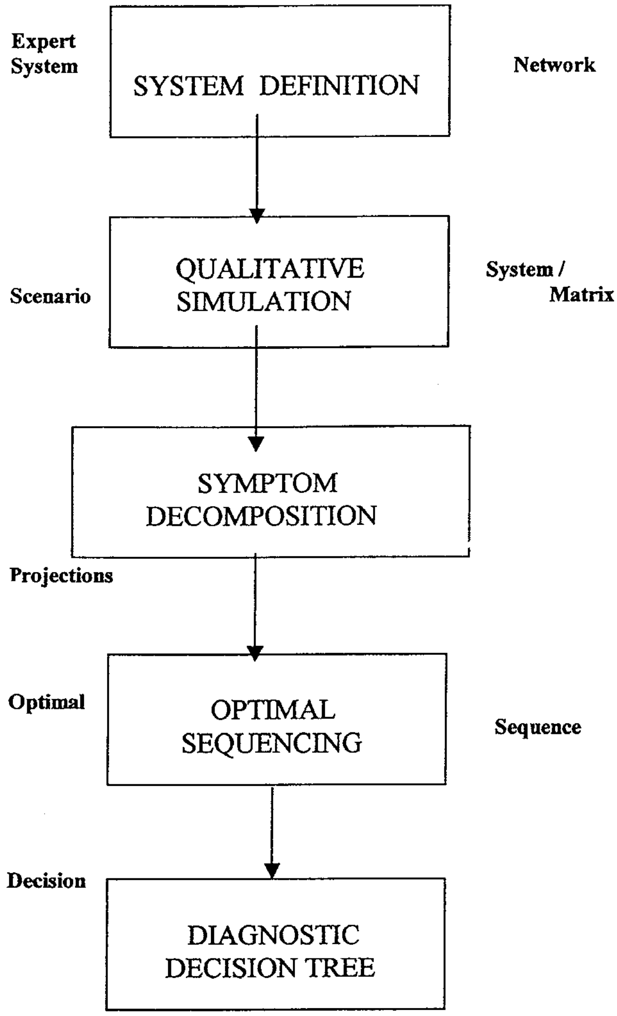

Figure 2. Qualitative model architecture

also the probability that each scenario or malfunction will take place. The quality of a structural relationship is determined through the entropy of the state transition matrix, which determines its forecasting power over a single step. The uncertainty (entropy) related to one input is calculated by:

$$H_i = -\sum_{O} p_i (O/I) \log_2 p_i (O/I) \quad (1)$$

where p(O/I) is the conditional probability of a certain output state (O), which occurs given that the input state (I) has already occured. The highest possible uncertainty (entropy) H_{max} is obtained when all probabilities are equal, and zero entropy is encountered for relationships that are totally deterministic. The overall uncertainty is then calculated as the sum:

$$H_m = -\sum p_i (I) H_i \quad (2)$$

where p(I) is the probability of that input occuring. The normalized overall uncertainty reduction H_r is defined as:

$$H_r = 1 - H_m / H_{max} \quad (3)$$

MEASURES OF THE QUALITATAVE INFORMATION VALUE

The currently employed methodology uses the ratio of observation, a quality measure. That reduces the mask quality if states exist that have been observed less than eight times. The observed ratio Q_r is introduced as an additional contributor to the overall quality measure.

$$Q_m = H_r Q_r \tag{4}$$

where

$$Q_r = (8e + 7d + 6j + 5s + 4m + 3k + 2l + 1i)/8n, \tag{5}$$

and n = number of legal input states, e = number of input states observed eight times, d = number of input states observed seven times, j = number of input states observed six times, s = number of input states observed five times, m = number of input states observed four times, k = number of input states observed three times; l = number of input states observed two times and i = number of input states observed only once.

If every legal input state has been observed at least eight times, Q_r is equal 1. If every legal input state has not been observed at all (no data are available), Q_r = 0. Thus, Q_r is then defined and can also be used as a quality measure. The overall quality of mask Q_m is then defined as the product of its uncertainty reduction measure and its observation ratio (Eq. (4)). The optimal sequences are calculating according to the following equation:

$$I_v = I_{v(new)} / \mathrm{cost} \tag{6}$$

$$I_{v(new)} = H = -\sum_{1}^{n} p_i \log_2 p_i \tag{7}$$

where, I_v is the information value, H the entropy of the new information value and p the probability of the scenario occurring. Equations (6) and (7) simply state that if the difference in the information between the scenarios is high, and the amount of time needed to observe this symptom is low, then the information value of the tested symptom is high [4,9].

Once a value has been calculated for all symptoms, the symptom with the best information value is chosen as the path head. An algorithm picks one of the values from this path head which filters out all scenarios which are not represented in the path head's projection. The projection is provided from the previous symptom decomposition stage [10]. This process is continued until the original group of scenarios is filtered down to one or until no symptoms exist which can differentiate the scenarios remaining. When any of these occur, the algorithm begins its filtering of the remaining subsets of scenarios branching off this initial path. In the final phase, the optimal sequence of symptoms is used to build a decision tree construction algorithm. This algorithm interprets the optimal sequence of events as similated in the previous algorithm and ships the results to an output file. The algorithm does this by following the paths, established in the optimal sequence tree, down in a depth first manner. It interprets various symptoms and scenarios found along the path and either issues a question, a causal branch, or a consequent scenario.

The output from each phase is sent to a summary file. After a complete qualitative simulation session, the file has five sections. First is a list of the components within the model where the input and output components are each specified by arrows toward and away from the components, respectively. Next the default state matrix is defined by a list of the input/output attributes, state variables, and meta variables for each component (database) with the default values for each specified. Following this comes the simulation result matrix. If steady state is never reached within in a particular scenario, a warning is given before the result matrix in which the scenario resides (decision mechanism). Each result matrix can display the results of all scenarios.

Subsequent results are shown in subsequent matrices.This section is followed by the symptom / scenario matrix. Finally, the resultant diagnostic decision tree for the management support system is presented.

DESCRIPTION OF THE CASE STUDY

In order to analyze the training of a qualitative simulator, a synthetic fiber production plant was examined (Figure 3). The process line for synthetic fiber (polycaprolactam) production consists of a chemical reactor, pump, two heat exchangers, three valves and seven streams.

The study of fault detection and diagnostics is concerned with designing a system that can assist a human operator in detecting and diagnosing equipment faults in order to prevent accidents. This interpretation and presentation means monitoring system symptoms.

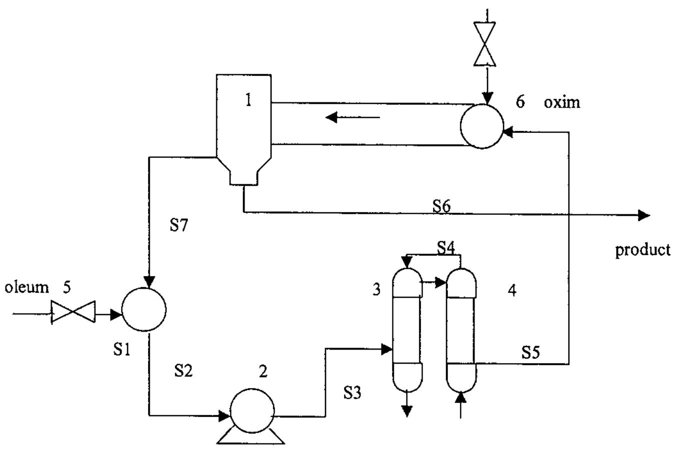

Figure 3. Scheme of the plant: 1 – reactor, 2 – pump, 3 and 4 – heat exchangers, 5 – inlet valve, 6 – outlet valve, S – stream

In the symptom decomposition phase, the relational symptom/scenario matrix is decomposed by using a projection operation to produce elementary relations.

This projection operation delineates which scenarios were found to have the same symptom values in their final state.

The original state matrix is given in Table 1. Table 2 gives changes made to the original model, which generates various scenarios of the considered process.

QUALITATIVE SIMULATOR DEVELOPMENT

The system topology or component interconnections are defined by the process connections of the working process model. The level of aggregation is defined by the modular component interconnections which define propagation paths of the attributes within the system. Attribute values are passed among system components via mediums. It is this propagation of attribute values by which system rules, when invoked recursively, generate the behavioral characteristics of the system.

Table 1. The original state matrix

Unit	Attribute state
Reactor(i)–flow	Medium
Reactor(i)–temp	Medium
Reactor(i)–press	Medium
Reactor(i)–state	Normal
Pump(i)–flow	Medium
Pump(i)–temp	Medium
Pump(i)–press	Medium
Pump(i)–state	Normal
Heat exchanger(i)–flow	Medium
Heat exchanger(i)–temp	Medium
Heat exchanger(i)–press	Medium
Heat exchanger(i)–state	Normal
Pipe(i)–flow	Medium
Pipe(i)–temp	Medium
Pipe(i)–press	Medium
Pipe(i)–state	Normal

Table 2. Scenario definition

Scenario	State changes
1	Process normal
2	Pump–malfunction
3	Reactor–leak
4	Heat exchanger preheater–block
5	Outlet pipe–leak
	Heat exchanger–leak
7	Valve–misoperation
	Reactor inlet pipe–block
9	Heat exchanger outlet pipe–leak

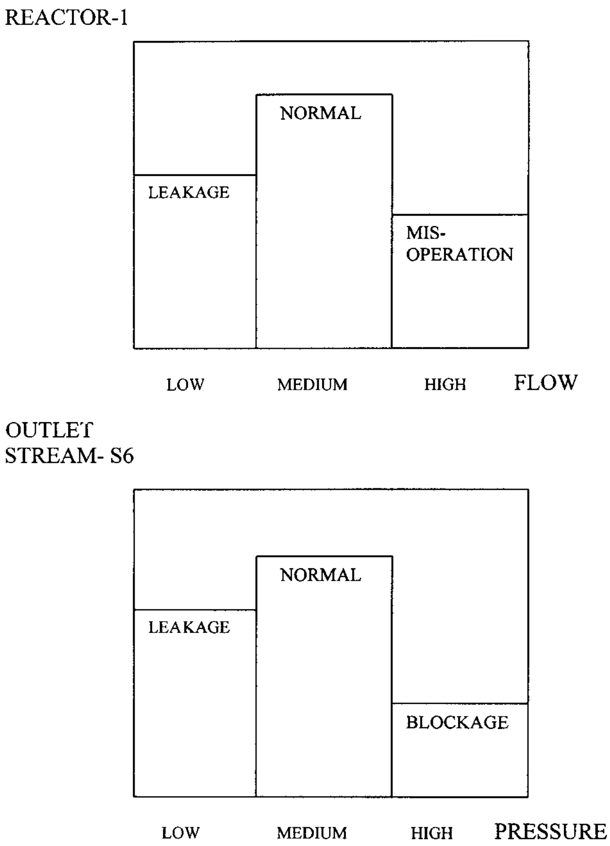

Figure 4. Analysis of the obtained results

The original model generates various scenarios [14]. In order to complete the qualitative simulation runs, a resultant symptom scenario matrix is formed. Faults and actions should correspond to changes in the state of equipment following deviations in the system variables. When leakage occurs in the upstream unit–USU, the influence of leakage on the USU cannot be removed by closing the equipment. However, when the leakage occurs in the downstream unit DSU, the influence of leakage on the DSU may be removed by closing the equipment. The model characteristics for the case study include 39 scenarios and approximately 720 rules. The Prolog programming language was chosen to develop the simulation model. Some of the outlet results are shown in Figure 4.

CONCLUSIONS

In the hypothesis stage a qualitative model of the system, combined with a library of phenomena, intelligently suggests phenomena which might explain the observed large system behavior. In the test stage these candidates are evaluated by building new models of the unit in question and comparing the resulting behavior with the observed deviations. The desired system must be general and flexible. The methodology should lead to a diagnostic system that can accommodate changes in the configurations. For any process system the components are regarded as the distinguishable parts within the system.

The additional measure of information value was introduced. The new qualitative information value was processed. The measure of qualitative information value was derived for the first time in this paper. The developed qualitative process simulator for fault diagnostics presented in this paper can serve as a useful support to system operators.

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NOTATION

I – input
H – uncertainty (entropy)
p – probability
O – output
Q – observed ratio

INDEX

m – overall
max – maximum
r – reduced

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IZVOD

KVALITATIVNI SISTEM ZA PODRŠKU UPRAVLJANJA HEMIJSKOG POSTROJENJA

(Naučni rad)

Jelenka B. Savković–Stevanović, Katedra za hemijsko inženjerstvo,
Tehnološko–metalurški fakultet Univerziteta u Beogradu, Beograd

Cilj ovog rada je da pokaže korisnost primene opšteg smisla kvalitativnog rezonavanja o procesu prikazanog modelom ljudskog ponašanja. Osnovna karakteristika kvalitativnog modelovanja i simulacije je opis kvalitativne varijable i logičkih pravila za manipulaciju vrednostima varijabli izmedju sistematskih stanja. Uvedena je dodatna mera kvalitativne informacione vrednosti. Ovaj rad je prvi izveštaj u literaturi koji pokazuje meru kvalitativne informacione vrednosti. Dobijeni rezultati ilustruju moć procene ponašanja sistema za vreme vanrednih situacija. Razvijeni kvalitativni simulator za dijagnostiku greške generiše originalne scenarije i pogodan je kao podrška operatoru za donošenje odluke.

Ključne reči: Simulacija ponašanja procesnih sistema • Kvalitativni procesni sistemi • Obrada kvalitativnih informacija • Kvalitativni simulator za otkrivanje poremećaja •
Key words: Process system behaviour simulation • Qualitative process support system • Qualitative information processing • Qualitative simulator for fault diagnosis •