Detecting Inverse Responses in Chemical Processes with Qualitative Simulation

S. Case*, Q. Shen*, R. Banares-Alcantara† and J. Ponton†
*Dept. of Artificial Intelligence, University of Edinburgh, UK
†Dept. of Chemical Engineering, University of Edinburgh, UK
{simonc, qiangs}@dai.ed.ac.uk, {rene, jwp}@chemeng.ed.ac.uk

Abstract

Operation of a chemical process requires the control of certain system variables. Prospective regulated variables should be tested to avoid inverse responses to a potential control adjustment. Design of such a process would therefore be facilitated if large ranges of system parameters could be simulated simultaneously, especially when the system description involves imprecise parameter and variable values. This paper presents an application of (fuzzy) qualitative simulation to this type of problem. It is shown why the use of pseudo-variables in the strict constraint-centred approach is impractical for simulating such systems. An alternative method for representing the system model, which enables the required simulations, is given. Despite the fact that qualitative ambiguity may cause spurious inverse responses to be generated, it is illustrated that if no qualitative inverse responses are produced then the physical system itself will not produce them either.

Introduction

In order to regulate complex industrial processes, the standard procedure is to select some measured variable or variables which correspond to the desired products, or are the desired products themselves. The control system can then use the current values of these measured variables to adjust the system variables so that the optimum amount of the desired product is produced. Ideally these variables would have a monotonic relation with respect to the quantity of desired product being generated over time, although this is not always possible. During the design of such a control system it is, therefore, important to know what types of behaviour a measured variable is capable of in order to ascertain what system parameters are appropriate for control.

Inverse responses are a class of behaviour often appearing in the control of chemical processes. The response of a regulated variable to a control adjustment is regarded as an inverse response if the sign of the difference between its original value (before the adjustment) and its final steady state (after the adjustment) differs from that between the original value and its initial response which immediately follows the adjustment. Figure 1 shows the typical behaviour of such a response. Variables which display an inverse response are difficult to control. Indeed, the usual procedure when automating control of a chemical process is to choose a measured variable which does not show inverse responses (Ponton 94).

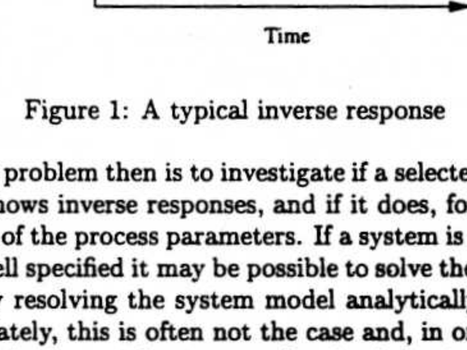

Figure 1: A typical inverse response

The problem then is to investigate if a selected variable shows inverse responses, and if it does, for what values of the process parameters. If a system is simple and well specified it may be possible to solve the problem by resolving the system model analytically. Unfortunately, this is often not the case and, in order to reveal the potential existence of such a behaviour, the physical process has to be simulated. The system may be simulated numerically given a differential equation model of the process, but this is only possible when the system parameters are precisely known. Furthermore, the simulation would only produce real number values for the initial state and parameters, whereas what is really required is that a *range* of values is simulated. Of course, an interval could be discretised so that regular points in the interval are simulated numerically, but a) this would be time-consuming, b) there would be no guarantee that all the possible types of behaviour had been simulated when the process possesses non-linear characteristics, and c) the behaviour in the boundaries between neighbouring intervals may not be precisely known.

This problem is further exacerbated by the lack of information available in the early stages of design. Typically, the system model may not be completely known: the relationships between variables may be approximately understood, but others may be missing. In addition, the control will probably have to occur over a large range of parameter values. For instance, in the reaction example given in section 2 of this paper, the parameter k_1 could have a large number of possible values. In designing a control system for this reaction the behaviour of the measured variable depends on this value. It is important, therefore, to know the behaviour of the measured variable for all the possible values of k_1. Indeed, at this stage the use of a precise value would be a hindrance (Dalle & Edgar 90).

Qualitative simulation algorithms are developed to simulate system behaviours non-numerically. The values taken by each variable are *symbolic* in some sense, and typically, system descriptions do not have to be complete. In particular, the fuzzy qualitative simulation algorithm, Fusim (Shen & Leitch 93), represents the variable values and parameters using fuzzy numbers. Such an algorithm could in fact simulate the physical system behaviour such that each simulation stands for an imprecise range of values. Therefore, *prima facie*, there is a very strong case for using Fusim to aid the design of chemical processes.

This paper is arranged as follows. The next section first gives an example of a real chemical process which shows inverse responses for some of its behaviours and then presents the general qualitative structure of inverse responses. Section 3 briefly describes Fusim and proposes a solution to the problems found when applying it to the real world application. These problems appear to be common to all qualitative simulation algorithms that follow the strict constraint-centred approach where the system model consists of constraints involving at most three arguments (so that the use of pseudo-variables may be necessary). Section 4 provides experimental results in comparison with those obtained by numerical simulations, thereby demonstrating both the advantages and the limitations of using fuzzy qualitative simulation to detect inverse responses. Finally, section 5 concludes the paper and points out important future work.

A Test Case

A good example of a real chemical process that may show inverse responses is the reaction scheme of Kravaris and Daoutides (see (Kravaris & Daoutides 90) and (Ponton 94) for details). Such a process may be numerically modelled by the following set of differential equations:

$$\dot{x}_1 = -k_1x_1 - k_3x_1^2 + (C_A^{in} - x_1)u$$
$$\dot{x}_2 = k_1x_1 - k_2x_2 - x_2u$$

Where: x_1 = concentration of A (the initial reagent, mol/l)
x_2 = concentration of B (the desired product, mol/l)
C_A^{in} = inlet concentration of A (mol/l)
u = flow-rate divided by reactor volume (mol/s)

To illustrate typical behaviours of such a process, as an example, given (in appropriate units): $k_2 = 100$, $k_3 = 10$, $C_A^{in} = 10$ and $u = 34.28$, and initial values of $x_1 = 3$, and $x_2 = 1.117$ the numerical behaviour over time of x_2 for different values of k_1 is shown in figure 2. Only the middle plot, where $k_1 = 50$ shows an inverse response.

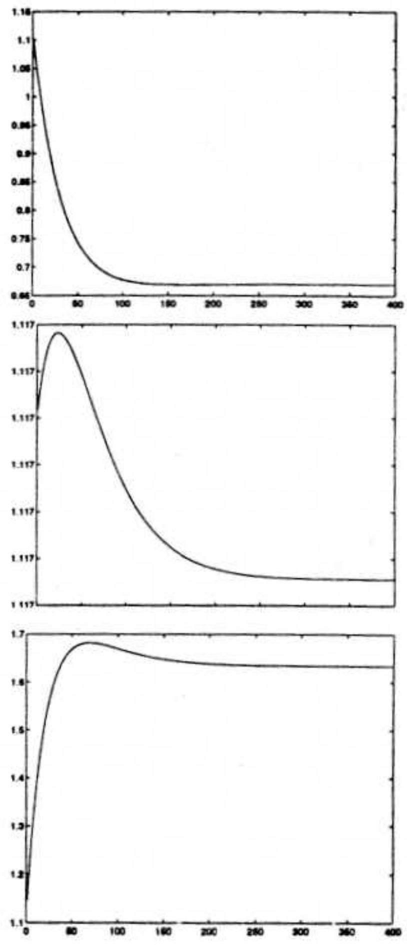

Figure 2: Behaviour of x_2 over time for k_1 = 25, 50, 100

This example demonstrates two important points about inverse responses. Firstly, inverse behaviours may only account for a small portion of all the possible behaviours. For this set of parameter values and initial values for the variables inverse responses were found for $49.998 < k_1 < 50.002$. Secondly, the scale of the inverse response may be tiny. When $k_1 = 50$, there is clearly an inverse response but both the initial height and the final depth are less than 0.001 mol/l.

Clearly, a system which could simulate the behaviours of the chemical process for ranges of the parameters would be extremely useful for detecting inverse responses. The system should be guaranteed to simulate all the possible behaviours of the chemical process, and then, using these simulations, to detect whether any of them does in fact constitute an inverse response.

Inverse responses are easily represented qualitatively, as shown in figure 3. The first two types initially increase (or decrease) by a qualitatively distinct amount, say ΔQ_{init}, then return to the initial value, and finally decrease by another amount ΔQ_{final}. The third and fourth types start with a derivative d_i but the magnitude stays at the same qualitative value until the derivative changes to the opposite sign to d_i. The last two types represent an inverse response whose underlying real-valued initial height (or depth) remains within the initial qualitative magnitude. From this it is clear that a qualitative behaviour can a) represent a large range of numerical behaviours and b) be readily tested for an inverse response.

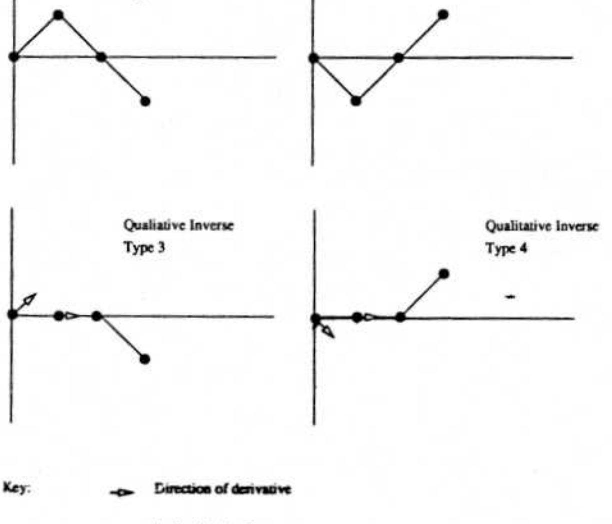

Figure 3: Qualitative representations of inverse responses

Qualitative simulation algorithms are guaranteed to generate all the possible behaviours of the physical system being simulated (Kuipers 86). Unfortunately, in general, all of them also generate *spurious* behaviours (Struss 88) which, loosely speaking, do not violate the qualitative system model but have no underlying real-valued counterpart. Consequently, a qualitative simulation algorithm may generate a behaviour which shows inverse response that the system being modelled may not actually have. Given this, it is important to note that a qualitative simulation cannot guarantee that if it detects an inverse response, then this behaviour will exist in the physical system. However it is guaranteed that if the qualitative simulation does not detect an inverse response, then no inverse response exists (for the parameter values and initial states given).

Detecting Inverse Responses with Fusim

In Fusim, system variables take values from a fuzzy quantity space consisting of fuzzy numbers. This quantity space is generated by a subjective but finite discretisation of the underlying numeric range of the variables. For computational efficiency, such qualitative values are characterised by the 4-tuple parametric representation (see later for example) of their membership functions within the implementation of the algorithm.

Fusim adopts a constraint-centred ontology in system-modelling: a model is represented by a set of fuzzy qualitative constraints. Possible values that variables can take are restricted by algebraic, derivative and/or functional constraints amongst them, with each constraint involving at most three variables. More specifically, the algebraic operations performed within a fuzzy quantity space are arithmetic operations among fuzzy numbers. A derivative constraint simply reflects that the qualitative value of a variable's magnitude must be the same as that of another variable's rate of change. Functional constraints are represented by fuzzy relations, thereby allowing imprecise and partial numerical information on functional dependencies between variables to be utilised.

When applied, Fusim takes as input a set of system variables, a set of constraints relating the variables (as the system model), and a set of initial qualitative states of the variables, and produces a tree of states with each path representing a possible behaviour of the system as output. In fact, Fusim first generates a set of possible transitions from one qualitative state description to its immediate successor states by exploiting the continuity of the variables. Further restrictions over these possible successor states are then imposed by a) checking for consistency with the definition of the constraints and the consistency between constraints which share an argument, b) checking for temporal consistency between variables' states via exploiting information on the rates of change of the variables, and c) checking for global consistency of the behaviour generated so far using additional knowledge about the system such as energy conservation. A detailed description of this simulation algorithm is, however, beyond the scope of this paper and can be found in (Shen & Leitch 93).

Whilst Fusim has been used successfully to simulate "toy" systems, it had not been tested against a real world application. Applying it to systems like the one given above prompted a main criticism which would also appear to apply to any strict constraint based qualitative simulation algorithm.

The problem was caused by ***pseudo-variables***. These variables are introduced to simulate the system using a composition of primitive (fuzzy) qualitative constraints that involve at most three arguments, which may be parameters or variables. This approach has been adopted because it is believed that any system can be represented by composing individual basic model-building blocks given its structural description. Being a constraint-centred approach, Fusim utilises a limited set of such basic blocks as indicated above. Describing the behaviour of a complex system will, therefore, often require additional variables that help to interrelate the primitive constraints. For example, to represent a system that may be modelled using the following ordinary differential equation (ODE):

$\dot{x} = -k_1 x - k_3 x^2 + (C_A^{in} - x)u$

Fusim has to employ seven pseudo-variables $pv1$ to $pv7$ so that the system can be described with the primitive fuzzy qualitative constraints below:

$(pv1 = k_1 * x)$ $\quad$ $(pv2 = x * x)$
$(pv3 = pv2 * k_3)$ $\quad$ $(pv4 = C_A^{in} - x)$
$(pv5 = pv4 * u)$ $\quad$ $(pv6 = pv5 - pv1)$
$(pv7 = pv6 - pv3)$ $\quad$ $(\dot{x} = pv7)$

However, in practice it was found that these pseudo-variables caused two related problems. The first problem was that the system model is constituted by many more variables than those used in its numerical counterpart. In the example above, apart from the parameters k_1, k_2, k_3, u and C_A^{in} the only variable in the ODE is x, whereas in the qualitative version there are eight variables. Given that the number of possible successor states from any given state is a maximum of 6^n in Fusim, with n being the number of variables used in the model (Shen & Leitch 92), the more variables there are the more possible future states will be generated. Thus, the strict constraint-based approach increases the time taken for a complete simulation of the system by increasing the value of n. There is however, a further problem which makes this approach impractical for a large-scale system. This is that for the majority of states their successors will only differ from the current state in the values of the magnitude or derivative of the pseudo-variables. In practice it was found that a "real" variable might well only change value once in five simulation steps. Since a minimum of three steps, each of which shows a change in the measured-variable, must be generated in order to detect an inverse response, then the simulation must be run to at least 15 steps ahead. Assuming that the average number of successors generated is 10 for each step, the simulation must then generate at least 10^{15} steps. This is obviously an extremely high figure and in practice it was not possible to run Fusim for long enough to detect an inverse response.

This problem will be most acute when there are a large number of parameters in the system model, since each parameter will require the introduction of a new pseudo-variable. Those systems which have no parameters, such as the mass on the spring under frictionless conditions, are immune to this criticism.

The solution proposed herein is that strict (fuzzy) qualitative constraints are replaced by compound constraints. Such constraints take the form of

left hand side $\cap$ right hand side

where $\cap$ signifies a fuzzy intersection. Given an ODE model, translating it to a qualitative one is therefore straightforward, without the need for the introduction of any pseudo variables which do not appear in the original ODEs. Following this proposal, for example, the counterpart qualitative constraint of the above ODE is represented by:

$\dot{x} \cap -k_1 x - k_3 x^2 + (C_A^{in} - x)u$

This renders pseudo-variables unnecessary and hence considerably limits the number of simulations that would otherwise have to be performed. On the other hand, Fusim still generates and filters states in the manner standard to all constraint-centred approaches and the system model still consists of a list of constraints. Moreover, when no exact numerical relationships are available, fuzzy relations can still be used to represent functional dependencies between system variables. This retains the ability to specify a physical system loosely and so the majority of the advantages of fuzzy qualitative simulation are still present.

This solution also gives a further advantage. In the original version of Fusim parameters are represented as variables whose derivative is always zero. Consequently they can only take their values from a pre-defined fuzzy quantity space. This has the disadvantage that to investigate differing intervals for these parameters the user may only alter the quantity or scalar assigned to the variable. This is a particularly awkward procedure if the user wishes to investigate intervals of widely varying sizes. However, in the revised version of Fusim parameters can be represented as a fuzzy-number whose values are particularly specified and independent of the quantity-space from which the system variables take their values. Consequently the relations between the behaviours of the variables and the parameters can be explored much more flexibly.

Experimental Results

Fusim was used to simulate several chemical processes (Case 96). This section concentrates on discussing the results obtained from simulating the process given in section 2. This is qualitatively modelled as follows:

$\dot{x}_1 \cap -k_1x_1 - k_3x_1^2 + (C_A^{in} - x_1)u$

$\dot{x}_2 \cap k_1x_1 - k_2x_2 - x_2u$

The behaviours generated were tested for inverse responses during simulation. If an inverse response was detected the simulation was stopped. The fuzzy initial values of the variables are characterised by the 4-tuple parametric representation as given in table 1. Within this table, for instance, the membership distribution $[2.0, 3.0, 0.5, 0.5]$ indicates that, with respect to the underlying numerical range of the variable x_1, real numbers falling within the interval $[2.0, 3.0]$ are regarded as a full member of the qualitative value (or the fuzzy set) termed *medium* and those within either $(1.5, 2.0)$ or $(3.0, 3.5)$ are assigned a partial membership, with any other real numbers having a null membership of *medium* (Shen & Leitch 93). The values for the parameters other than k_1 were set to the following real numbers: $k_2 = 100$, $k_3 = 10$, $u = 34.28$, $C_A^{in} = 10$. The parameter k_1 itself was given varying interval values in order to investigate its impact on the system's behaviour.

Variable	Initial Value	Membership Distribution
x_1	*medium*	$[2.0, 3.0, 0.5, 0.5]$
x_2	*large*	$[1.125, 1.35, 0.225, 0.075]$

Table 1: Initial values

To verify the results Matlab was used to simulate the ODEs given in section 2 as a "gold-standard". When running the numerical simulations with Matlab an interval value was discretised so that regular points in the interval, including the two boundaries, were simulated. For the present application, since all possible inverse responses should be detected, a fuzzy interval was treated as a crisp one defined by its two extremities. Using Matlab inverse responses were found for $50.3 < k_1 < 89$. It is important to note that this is different from the limits found in section 2 because the initial states of the variables are *intervals* not real numbers. The presence of an inverse response depends on the initial values of the variables as well as the parameters.

Fusim's results are summarised in table 2. Initially Fusim finds inverse responses for $40 \leq k_1 \leq 80$. By narrowing the sizes of the intervals it can be seen that Fusim finds inverses for $49 < k_1 \leq 75$. At the lower end of the range of k_1 Fusim detects inverse responses where they exist, but then also for $49 < k_1 < 50$ where numerically they cannot be found. This is due to spurious behaviours being generated. At the upper bound Fusim fails to detect inverse responses for $k_1 > 75$. This was due to the fact that the derivatives in the initial state only reflected some of the possible initial states for this set of initial magnitudes of parameters. Consequently certain behaviours were not being simulated. Subsequent tests demonstrated that when the process was simulated from all the admissible initial states inverse responses could be found for $k_1 \leq 90$.

In summary then Fusim found inverse responses for $49 < k_1 \leq 90$, which demonstrates that for this example it is able to find inverse responses when they exist, and only generates spurious inverse responses for values of k_1 close to the numerically discovered boundaries of the existence of inverse responses. This is natural due to the fact that only imprecise information is available on these boundaries.

Sample qualitative behaviour graphs showing the behaviour of x_2 for varying values of k_1 are given in figure 4. Each integer x-value on a graph corresponds to a step of the simulation, whilst the y-values show the fuzzy qualitative magnitude of x_2 at that step. Additionally, the labels on the graph show the fuzzy qualitative value of the derivative of x_2 at that step. It can be seen that for the interval $40 \leq k_1 \leq 60$ the qualitative graph is a *qualitative inverse* of type 3 as shown in figure 3. The other two behaviours do not represent any type of inverse response. Comparing these qualitative graphs with the numerical graphs shown in figure 2 it is clear that these behaviours have been simulated by Fusim.

Interval	Time	Inverse Found	No. of Behaviours
0-40	4157s	No	21,223
40-60	2.86s	Yes	n/a
60-70	82s	Yes	n/a
70-80	83s	Yes	n/a
80-90	208s	No	663
40-50	130s	Yes	n/a
50-60	82s	Yes	n/a
40-46	257s	No	911
45-47	255s	No	911
45-48	257s	No	911
45-49	257s	No	911
49-50	130s	Yes	n/a
50-50	3s	Yes	n/a
70-75	83s	Yes	n/a
72-75	83s	Yes	n/a
71-75	83s	Yes	n/a
73-75	83s	Yes	n/a
74-75	83s	Yes	n/a
75-76	229s	No	945
75-80	230s	No	945

Table 2: Results for various interval sizes of k_1

These results, together with others obtained so far

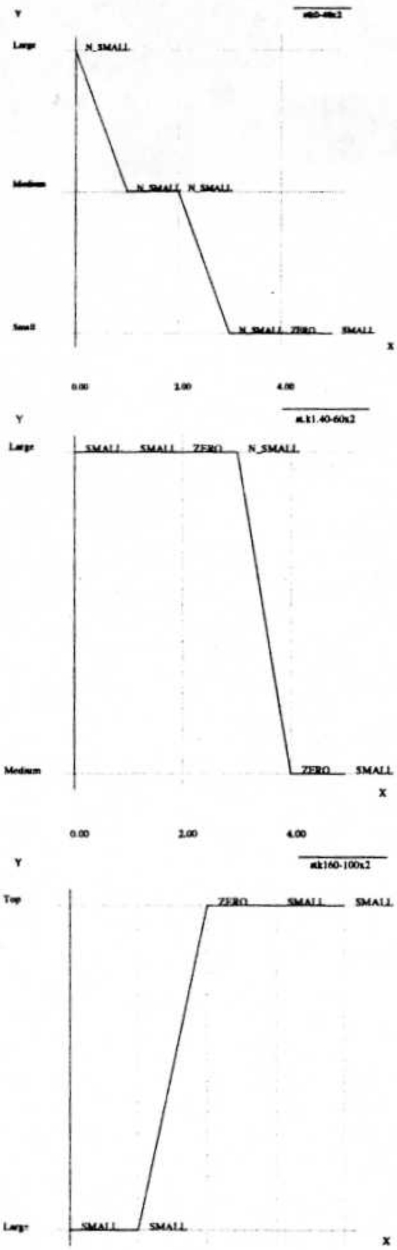

Figure 4: Sample qualitative behaviours of x_2 over time (for $0 \leq k_1 < 40$, $40 \leq k_1 \leq 60$ and $60 < k_1 \leq 100$)

using different system models (Case 96), demonstrate that if Fusim does not find an inverse response then there is no inverse response. Furthermore, it appears that spurious inverse responses are in general only generated near to the limits of the numerical presence of inverse responses (e.g. in the case of $49 < k_1 < 50$).

Conclusion and Future Work

This paper purports to show that the fuzzy qualitative simulation algorithm, Fusim, can be used to simulate real-world systems, in particular to aid the design task of chemical processes that have the potential to exhibit inverse response behaviours. In order to achieve this, however, it is necessary to alter the method of describing the system such that the constraints are no longer strict (fuzzy) qualitative constraints, as used in conventional constraint-centred qualitative simulations. Such a method is proposed in the paper.

This revised algorithm can be used to show that for a given set of parameters a system model will not display any inverse responses. It is also possible to alter the parameter values independently of the quantity-space so that the limits where inverse responses occur can be more closely approximated.

The results so far have been very promising. However, the alterations to the standard version of Fusim have not yet been investigated in depth and the work has been applied to only a limited number of examples. A planned next step is to establish a formal description of the revised algorithm and to examine if it possesses properties such as soundness and completeness. Further work will include applying this algorithm to more complex models.

From the point of view of detecting inverse responses, the present version of Fusim blindly simulates the whole behaviour tree for the specified number of steps, effectively making a depth-first search. However, it can be shown that after a certain point some of the simulated branches will not show any inverse responses. It would be more efficient if Fusim made a more intelligent search of the behaviour tree such that obviously fruitless branches were ignored at the earliest possible opportunity. This would enable simulations to be run to more steps. It is also worth indicating that, for the simulations carried out so far, only some of the possible initial (fuzzy qualitative) states for a process had been investigated. Work should be done on the automatic generation of all the possible initial states with respect to a given process, so that a complete picture of it can be revealed to detect whether or not an inverse response would be present within its entire operating range.

References

S. Case. Using Fusim to detect inverse responses. Project report, Dept. of Artificial Intelligence, University of Edinburgh, 1996.

D. Dalle and T. Edgar. Qualitative modelling of chemical reaction systems. In M.L. Mavrovouniotis, editor, *Artificial Intelligence in Process Engineering*, pages 1–36. Academic Press, 1990.

C. Kravaris and P. Daoutides. Nonlinear state feedback control of second-order nonminimum-phase nonlinear systems. *Computers and Chemical Engineering*, 14:439–449, 1990.

B. Kuipers. Qualitative simulation. *Artificial Intelligence*, 29:289–338, 1986.

J. Ponton. Detecting inverse responses in process models. 1994-01, Dept. of Chemical Engineering, University of Edinburgh, 1994.

Q. Shen and R. Leitch. On extending the quantity space in qualitative reasoning. *Artificial Intelligence in Engineering*, 7(3):167–174, 1992.

Q. Shen and R. Leitch. Fuzzy qualitative simulation. *IEEE Transactions on Systems, Man and Cybernetics*, 23(4):1038–1061, 1993.

P. Struss. Mathematical aspects of qualitative reasoning. *Artificial Intelligence in Engineering*, 3(3):156–169, 1988.