Qualitative Simulation of Chemical Process Systems: Steady-State Analysis

A method of qualitative simulation for continuous process systems that predicts the steady-state measurement patterns generated as a result of process malfunctions is presented. The method is based on qualitative versions of the steady-state process equations and requires no numerical information beyond the signs and relative values of certain groups of parameters. Previous methods of qualitative simulation (Umeda et al., 1980; de Kleer and Brown, 1984; Forbus, 1984; Kuipers, 1986) have tended to generate multiple solutions that do not coincide with any observable system behaviors. In the current method, spurious solutions are reduced using "latent" constraints associated with analytically redundant model equations, and "nonlatent" constraints based on causality, and derived from the extended signed directed graph (ESDG). The ESDG is similar to the signed directed graph (SDG) (Iri et al., 1979), but includes certain nonphysical branches that account for complex dynamics (inverse and compensatory response due to negative feedback). Necessary conditions based on the topology of the SDG for the occurrence of complex dynamics are developed. Based on these criteria, assumptions concerning disturbance propagation are introduced that minimize spurious interpretations of system behavior while guaranteeing inclusion of the steady-state response. The method is demonstrated by simulating the effects of equipment malfunctions on a model process.

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Introduction

The operators of process plants are responsible for various supervisory control activities including the implementation of start-up, shut-down and change-over procedures, process monitoring, and malfunction diagnosis. The operator's task in the event of a process disturbance or malfunction is to diagnose the cause of the plant upset quickly and accurately so that corrective action may be taken. Studies of human diagnostic strategies indicate that a hypothesis/test strategy is frequently used in diagnosis (Rasmussen, 1980). From the observed patterns of deviations, the operator hypothesizes a potential cause of the upset. The operator then mentally simulates the effect of the hypothesized malfunction on process behavior. If the simulated behavior matches observed behavior, the hypothesis may be retained; otherwise, an alternative hypothesis may be formed. It has been suggested that, due to the high cognitive load on the operator to generate a set of symptoms to test a hypothesis, the use of computers during the hypothesis/test cycle should be considered (Rasmussen, 1980).

There is a motivation in this context to avoid the effort and expense of creating, maintaining, and computing with rigorous dynamic mathematical models of large-scale processes by focusing on qualitative indicators of process condition such as alarm order and high/low measurement patterns. This philosophy has been adopted in many previous attempts to address the problem of disturbance analysis in complex processes (Andow and Lees, 1975; Iri et al., 1979; Long et al., 1980; Bastl and Felkel, 1980; Martin-Solis et al., 1982; Danchak, 1982; Tsuge et al., 1985a). Yet little fundamental work on qualitative modeling of disturbance propagation in chemical plants has been done, several exceptions being Umeda et al. (1980), Andow et al. (1980), Lees (1984), and Dalle Molle and Edgar (1987). Other studies of qualitative modeling are currently being conducted in the field of artificial intelligence; a useful compilation of this research given in Bobrow (1985a).

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Previous methods of qualitative modeling have tended to suffer from excessive generation of multiple solutions, which could lead to a loss in diagnostic resolution if these methods were used in malfunction diagnosis. These solutions (also known as interpretations) fall into two classes: i) realizable behaviors, which correspond to an actual qualitative behavior in the class of devices (systems that have identical qualitative descriptions and differ only in quantitative parameter values are considered to be members of the same qualitative class); and ii) spurious behaviors, not exhibited by any quantitative realization of the system. Spurious solutions are generated when competing qualitative influences cannot be resolved, for example when one factor tends to make a variable increase, and another tends to make it decrease. Kuipers (1986) has proven that qualitative simulations in general cannot be guaranteed to exclude spurious solutions, however several strategies for reducing spurious solutions have been pursued. DeKleer (1979) recommends the use of quantitative and teleological (design purpose) information to resolve ambiguities in qualitative models. Raiman (1986) uses order of magnitude information to reduce some of the ambiguity. No method of resolving ambiguous qualitative influences is offered by the Qualitative Process Theory of Forbus (1984) and the signed directed graph (Iri et al., 1979; Umeda et al., 1980).

The major significance of the current paper is that we extend previous methods of qualitative modeling by providing a systematic method of reducing the number of spurious solutions in qualitative modeling. We show that spurious solutions can be largely eliminated using qualitative information, without appeal to quantitative or teleological information. The problem considered is qualitative malfunction simulation of continuous systems. Specifically, for a given malfunction or malfunctions, we attempt to determine the ultimate (steady-state) direction of deviation of system state variables relative to their nominal steady-state values. Thus, the relevant qualitative values for each variable are high (+), low (−), and normal (0). For simplicity, we do not concern ourselves with additional landmark values (Forbus, 1984), nor with the prediction of dynamic trends (Dalle Molle and Edgar, 1987), which would require a richer description of the state space.

The view of qualitative process behavior advanced in this paper is that the effects of faults are causally propagated from one variable to another, ultimately satisfying steady-state process constraints. These constraints are sets of algebraic equations, represented qualitatively as steady-state confluence equations (de Kleer and Brown, 1984). Causality is represented by the extended, signed, directed graph (ESDG), which captures the basic causal principle that effects must be propagated locally within the topology of a system (Bobrow, 1985b).

Within this framework, ambiguities are reduced by the introduction of "latent" and "nonlatent" constraints. Latent constraints are derived from two principal sources: redundant process equations derived by algebraic manipulation of a basic set of independent equations, and constraints imposed by causality, which may be difficult to derive by algebraic manipulation. Nonlatent constraints are derived from causal considerations and help to eliminate responses associated with unstable steady states.

In the following, the two integral components of the fault simulation methodology are introduced: confluences and the ESDG. An extended example of qualitative simulation is also presented. In addition, performance of the method with respect to resolving ambiguities is discussed.

Simulation of Steady States by "Pure" Confluences

Quantitative mathematical models of continuous process systems consist of simultaneous algebraic and differential equations. In the steady-state limit, these models can be reduced to algebraic equation models, derived by discretization or lumping of spatial dimensions in the case of distributed systems. In this section, we show how algebraic equations provide qualitative constraints (confluences) on the ultimate direction of change of system variables.

Basic steady-state constraints

The quantitative model describing a system at steady state can be expressed as a set of n independent (basic) nonlinear equations

$$\underline{f}(\underline{x}, \underline{u}, \underline{p}) = \underline{0}; \quad \underline{x} = \underline{x}_0, \underline{u} = \underline{u}_0, \underline{p} = \underline{p}_0 \tag{1}$$

where $\underline{x}$ is a vector of n-independent state variables, $\underline{u}$ and $\underline{p}$ are vectors of externally specified variables (inputs) and system parameters, respectively. Because of the possibility of algebraic manipulation, this set of equations is not unique. Typically in formulating the model, the modeler writes equations that refer to particular units or subsystems so that each equation is local and does not involve variables in nonadjacent subsystems.

Disturbances and malfunctions can be represented by perturbations of one or more of the inputs, $\underline{u}$ or parameters, $\underline{p}$ from their nominal steady-state values. For a finite perturbation, the change in the system can be expressed as:

$$\int \partial \underline{f}/\partial \underline{x} \cdot d\underline{x} + \int \partial \underline{f}/\partial \underline{u} \cdot d\underline{u} + \int \partial \underline{f}/\partial \underline{p} \cdot d\underline{p} = \underline{0}, \tag{2}$$

where the lower and upper limits of integration are the initial and final steady states, respectively. Applying the mean value theorem, Eq. 2 becomes:

$$\partial \bar{\underline{f}}/\partial \underline{x} \cdot \Delta \underline{x} + \partial \bar{\underline{f}}/\partial \underline{u} \cdot \Delta \underline{u} + \partial \bar{\underline{f}}/\partial \underline{p} \cdot \Delta \underline{p} = \underline{0} \tag{3}$$

where $\partial \bar{f}/\partial i$ is the mean value of the partial derivative along the integration path. Steady-state confluences can be derived by qualitative translation of Eq. 3:

$$[\partial \bar{\underline{f}}/\partial \underline{x} \cdot \Delta \underline{x}] + [\partial \bar{\underline{f}}/\partial \underline{u} \cdot \Delta \underline{u}] + [\partial \bar{\underline{f}}/\partial \underline{p} \cdot \Delta \underline{p}] = \underline{0} \tag{4a}$$

The square brackets [·], represents the qualitative value (sign) of the argument. The operations of qualitative algebra are defined in Table 1. Note that addition of quantities of opposite sign results in ambiguity, since relative magnitudes are not known. Under the rules of qualitative algebra, Eq. 4a is equivalent to:

$$[\partial \bar{\underline{f}}/\partial \underline{x}] \cdot [\Delta \underline{x}] + [\partial \bar{\underline{f}}/\partial \underline{u}] \cdot [\Delta \underline{u}] + [\partial \bar{\underline{f}}/\partial \underline{p}] \cdot [\Delta \underline{p}] = \underline{0} \tag{4b}$$

In order to maintain consistency with the notation of de Kleer and Brown (1984), Eq. 4b is rewritten as

$$[\partial \bar{\underline{f}}/\partial \underline{x}] \cdot [d\underline{x}] + [\partial \bar{\underline{f}}/\partial \underline{u}] \cdot [d\underline{u}] + [\partial \bar{\underline{f}}/\partial \underline{p}] \cdot [d\underline{p}] = \underline{0} \tag{4c}$$

Table 1. Tables of Qualitative Operations

$[dx] + [dy]$

$[dx]$ / $[dy]$	+	0	−	?
+	+	+	?	?
0	+	0	−	?
−	?	−	−	?
?	?	?	?	?

$[dx] - [dy]$

$[dx]$ / $[dy]$	+	0	−	?
+	?	−	−	?
0	+	0	−	?
−	+	+	?	?
?	?	?	?	?

$[dx] \cdot [dy]$

$[dx]$ / $[dy]$	+	0	−	?
+	+	0	−	?
0	0	0	0	0
−	−	0	+	?
?	?	?	?	?

$[dz] = \delta([dx])$

$[dx]$	+	0	−	?
$[dz]$	0	+	0	+ or 0

where the differential, d, refers to a total macroscopic rather than an infinitesimal change in a quantity.

Equation 4c is a set of equations that are sums of products of parameter/variable relationships (partial derivatives) and differential quantities, also known as "mixed" confluences (de Kleer and Brown, 1984). These can be converted to a set of "pure" confluences (a simple sum of differential quantities) by assigning fixed signs to the partial derivatives. This is done by defining a set of inequality constraints $\underline{C}$ under which the partial derivatives in Eq. 2 possess the same signs as at the initial state. Usually, detailed numerical information is not required in determining signs of the partial derivatives, as they are determined from signs of ordinal relationships (e.g., pressure drops, relative temperatures, concentrations). (If the signs cannot be determined unambiguously, the confluence is omitted since no useful information is provided.) Within $\underline{C}$, the average values of the derivatives in Eq. 4c have the same sign as the partial derivative at the initial state. The ranges of state variables and parameter values which satisfy these inequalities define the range of validity of the "pure" confluences, i.e., the scope of the system's qualitative class.

The functional relationships in Eq. 1 do not have to be completely specified in order to derive confluences. (Further references are to "pure" confluences, and the distinction between "pure" and "mixed" confluences is now dropped.) For example, the equation which describes the flow of liquid for all classes of control valves is:

$$F = f^{+}(V, |P_I - P_O|) \cdot (P_I - P_O)/|P_I - P_O| \qquad (5)$$

where f^{+} is an unspecified monotonically increasing function of the valve stem position, V, and the absolute pressure difference, $|P_I - P_O|$. For forward flow, $(P_I > P_O)$, the confluence derived from this equation, independent of the exact nature of f^{+}, is

$$[dF] = [dP_I] - [dP_O] + [dV] \qquad (6)$$

Equation 6 states that a positive change in flowrate cannot occur without either a positive change in inlet pressure or valve stem position, or a negative change in outlet pressure. This confluence is a logical constraint on the behavior of the valve, and not an indication of causality. Causality cannot be construed from this equation, as increased flow would not cause opening of the valve, but could result in increased downstream pressure.

During a transient, the inequality conditions $\underline{C}$ defining the qualitative class can be violated, leading to a transition between qualitative regimes. These transitions can only occur when conditions defining the validity of some process equations in Eq. 1 no longer hold or some partial derivatives in Eq. 4c change sign. Typical qualitative transitions are phase changes, flow reversals, and controller saturation. The problem of identifying potential class transitions has been addressed by de Kleer and Brown (1984), Forbus (1984), Kuipers (1984), and Williams (1984). At best these analyses provide a partial ordering but do not determine which transitions actually occur, since this determination usually requires numerical information. Determining the set of actual transitions is a problem that is not addressed in this work, and it will be assumed that the only allowable transition between qualitative regimes is the saturation of control loops.

The set of confluences (Eq. 4c) form a set of inherently simultaneous qualitative equations. A combination of constraint satisfaction and generate and test is used to find all possible solutions to the system of confluences. All qualitative patterns of variables that satisfy every confluence in the set are feasible solutions. An algorithm for solving systems of confluences is provided as supplementary material.

In testing a confluence, appearance of the ambiguous value, (?), automatically satisfies the confluence. The consequence of this ambiguity is that a set of n-independent confluences in n unknowns is not guaranteed to yield a unique solution. If ambiguities cannot be resolved within a set of confluences, multiple solutions result. The set of values, (+, 0, −), do not form an algebraic group under qualitative algebraic operations, therefore there is no general theory for prediction of solution uniqueness or multiplicity.

Resolving ambiguity with latent constraints

In cases of multiple interpretations, some of the solutions to the system of independent confluences may be spurious while others may be genuine and occur for certain quantitative realizations of the system's qualitative class. In this section, a procedure for reducing the number of spurious interpretations using "latent" constraints is outlined.

Latent constraints are confluences derived from redundant algebraic quantitative process equations and from causal considerations. Because qualitative arithmetic in general requires more equations than unknowns to generate unique solutions, it is usually necessary to begin with an overspecified set of quantitative equations to get a fully determined set of confluences.

As a general rule, redundant equations containing no more, but preferably fewer, nonzero variables than the independent equations from which they are derived are most useful in eliminating spurious solutions. This is because the greater the number of nonzero terms in a qualitative equation, the more likely that addition of terms will yield ambiguity. No ambiguity is possible in confluences containing one or two variables.

The number of potential latent constraints that can be derived from a set of n-independent equations (unknowns) can be estimated as follows. The number of ways to select r variables from n is $C(n, r) = n!/(n-r)!r!$. If a particular selection of r variables is made, $n - r$ variables are eliminated from the original set, resulting in a subset of r-independent equations in r variables. For each unique selection of r variables, at least one new confluence can always be obtained. Assuming just one confluence from each selection of r variables, a conservative lower bound (for sparse systems of equations, a lower estimate is obtainable) on the number of latent confluences that can be derived from algebraic manipulation of a set of n-independent equations is the sum from $r = 1, \ldots n$, less the number of independent equations:

$$C(n, 1) + C(n, 2) + \ldots + C(n, n) - n = 2^n - n - 1 \qquad (7)$$

Thus, the number of possible latent constraints increases exponentially with the number of unknowns.

Equation 7 shows that equations involving one unknown (i.e., the analytical solution) are included in the set of redundant equations. Thus, if an analytical solution exists, the redundant set of noncausal, steady-state confluences is theoretically able to provide the ultimate qualitative response from all (stable and unstable) steady states without other interpretations. However, because analytic complexities arise quickly in the attempt to derive useful latent constraints, and due to the large number $[O(2^n)]$ of potential latent constraints, it may be extremely difficult to derive all the necessary latent confluences to achieve this degree of resolution. As yet we have no general method of determining *a priori* how many or which latent confluences are required to eliminate solutions not in the set of stable and nonstable steady states. A heuristic approach to deriving useful latent constraints has proved useful.

The following heuristics have been employed to guide the search for useful latent constraints:

a) *Global balances for conserved quantities.* Because of the ambiguity of qualitative arithmetic, qualitative balances for conserved fundamental quantities (e.g., material and energy) around subsystems of a process do not assure conservation of the quantities in the overall system. Equation 10 is a latent confluence of this type.

b) *Compatibility relationships.* These confluences derive from equating driving forces around loops for potential-driven flows. Confluences derived from pressure compatibility relationships in bypass or recycle loops (Eq. 11) are examples of this type.

c) *Balances from bilinear conservation relationships.* Some conserved quantities (e.g., energy) are usually expressed as products of extensive (mass or volume) and intensive (e.g., temperature) variables. Eliminating one of the extensive variables (by using a total balance around a process subsystem) from bilinear conservation equations often results in useful confluences.

d) *Elimination of groups of variables.* Characteristic groupings of variables often occur in equations, for example, for rates of reaction and heat duties. Elimination of these groups can result in useful latent confluences, especially when the resulting equation contains fewer variables than the original equations. A confluence obtained by eliminating the reaction rate expression from the mass balance and energy balance in a nonisothermal, continuous stirred tank reactor is an example of this type of latent confluence.

e) *Causal constraints.* The requirement of causality adds two types of constraints on the behavior of the system. First, causality provides latent constraints that may otherwise be difficult to derive from the independent equation set. Second, causality provided new constraints, not latent in the set of steady-state algebraic equations, which help eliminate responses from unstable steady states, as will be discussed later.

Tradeoff between modularity and multiplicity

Strategies a) and b) for deriving latent constraints point up a very important limitation in qualitative modeling involving modularity. Modularity is the property that the behavior of a system can be deduced from the behavior of the components of the system. In conventional modeling of chemical engineering systems, the ability to divide a process into unit operations has been an extremely useful concept which has led to, among other things, modular flowsheet simulation programs. A similar property would be desirable in qualitative modeling.

In the subsequent example, it will be seen that satisfaction of qualitative mass balances on process subsystems does not automatically result in satisfaction of the qualitative mass balance on the combined system. Similarly, qualitative pressure drop relations at the local or subsystem level do not guarantee pressure compatibility at the global level across recycle or bypass loops. Omission of "global" latent constraints of types a) and b) can result in generation of spurious interpretations of system behavior. Therefore, in qualitative modeling, there is a trade-off between modularity and solution multiplicity.

A possible "fix" of this problem could be achieved if latent constraints could be generated automatically. There are a number of symbolic algebra computer packages that could be helpful in this regard. A qualitative flowsheeting system storing the local confluences and the analytic component models could automatically generate the global latent confluences corresponding to particular flowsheet topographies, while the overall system would retain an appearance of modularity. However, automatic generation of latent confluences is beyond the scope of the current research.

Example of simulation using noncausal confluences

Figure 1 shows a simple recycle loop with fixed boundary pressures. A constant speed centrifugal pump maintains recycle

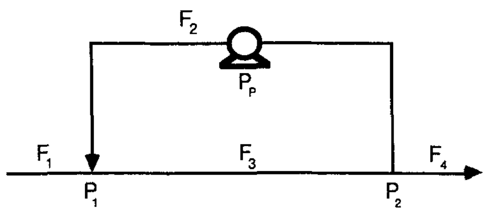


Figure 1. Recycle loop in the example.

flow. The head delivered by the pump, P_p, decreases with increasing flow. The local (basic) steady-state confluences for this system are:

$$[dF_1] + [dP_1] + [dR_s] = 0, [dR_s] = (0) \quad (8a)$$

$$[dF_2] = [dP_2] + [dP_p] - [dP_1] \quad (8b)$$

$$[dF_3] = [dP_1] - [dP_2] \quad (8c)$$

$$[dF_4] = [dP_2] \quad (8d)$$

$$[dF_1] + [dF_2] = [dF_3] \quad (8e)$$

$$[dF_2] + [dF_4] = [dF_3] \quad (8f)$$

$$[dP_p] + [dF_2] = 0 \quad (8g)$$

This is a system of eight equations in eight unknown variables that would have a unique solution in the quantitative domain. A partial blockage in pipe 1 is represented as a change in flow resistance, R_s of the pipe. This modifies Eq. 8a to:

$$[dF_1] + [dR_s] + [dP_1] = 0, [dR_s] = (+) \quad (9)$$

There are 11 solutions to Eqs. 8b–g and 9, Table 2.

Two latent confluences are required to achieve a unique solution. These are,

$$[dF_1] = [dF_4] \quad (10)$$

from an overall mass balance, and

$$[dF_2] + [dF_3] = [dP_p] \quad (11)$$

Table 2. Solutions to Local Confluences of Recycle Loop for Partial Blockage in Pipe 1

Solution	F_1	F_2	F_3	F_4	P_1	P_2	P_p
1	–	+	–	–	–	–	–
2	–	+	+	+	+	+	+
3	–	–	–	+	+	+	+
4	+	+	+	–	–	–	–
5	0	+	+	–	–	–	–
6	+	–	–	–	–	–	+
7	0	–	–	–	–	–	+
8	–	0	–	–	–	–	0
9	–	+	+	–	–	–	–
10	–	+	0	–	–	–	–
11	–	–	–	–	–	–	+

from the pressure compatibility relationship around the recycle loop. Equation 11 is derived from elimination of the pressure difference, $P_1 - P_2$, from the flow equations for F_2 and F_3. The first row in Table 2 is the only solution that satisfies both latent confluences. Thus this solution is the only possible behavior of the system and is valid for all numerical realizations of parameter values.

Using Casual Information in Steady-State Simulation

Cause-and-effect arguments are a basic component of human reasoning about system behavior (Bobrow, 1985b). However, modeling of causality in previous works on qualitative simulation has been problematic. Forbus (1984) dismisses causality as "mainly a tool for assigning credit to hypotheses for observed or postulated behavior." De Kleer and Brown (1984) use a concept of causality that describes transients during mythical (infinitesimal) time instants when noncausal confluences are not valid. Causality is not represented explicitly but is discovered by a set of heuristics during constraint propagation among confluences. Iwasaki and Simon (1986) present a theory of causality, in which causality is construed as output set assignment (Steward, 1962) of a set of simultaneous algebraic equations. Starting with assumed exogenous variables and the noncausal model of the process, they attempt to deduce local causality using precedence ordering that provides the order by which subsets of variables can be solved for by direct substitution. This procedure is incomplete at best as it does not provide causal ordering among variables in feedback loops.

Iri et al. (1979) introduce the single-stage signed directed graph (SDG). This representation provides explicit causal relationships among variables (including those in feedback loops). Umeda et al. (1980) extend this representation to multiple stages to handle qualitative dynamic simulation. Shiozaki et al., (1985) and Tsuge et al. (1985b) extend the possible qualitative values of variables in the SDG to a five-range pattern (+, +?, 0, –?, and –) to deal with states that are outside the range of normal process variability but still within predetermined threshold limits. The Lapp and Powers (1977) digraph is essentially similar to Iri's. The explicit representation of causality provided by digraphs is most useful and is addressed in this work.

The SDG and rules for disturbance propagation using the SDG will be reviewed, as well as limitations of the propagation assumptions. The previous SDG method excludes the ultimate response in certain systems, in which variables exhibit types of complex dynamics, namely inverse and compensatory responses. [Inverse response is defined as a pattern where the final (steady-state) sign of a variable is opposite from the initial direction of deviation of the variable. Compensatory response occurs when the variable returns to its nominal steady-state value after an initial deviation.] Necessary conditions related to the topology of the SDG, under which the SDG excludes ultimate process behavior are described. From these criteria, an extension to the SDG, the extended signed directed graph (ESDG), is developed, and then we present a procedure for converting the ESDG into a set of confluences governing the qualitative steady-state response of the system. Finally, examples demonstrating how additional causal confluences derived from the ESDG eliminate spurious interpretations produced by noncausal confluences are presented.

Single-stage signed directed graph

The SDG is causal model of a process consisting of nodes, symbolizing process variables (parameters), and signed directed branches representing immediate local cause-and-effect relationships between variables. Nodes in the SDG assume the qualitative values (0), (+), and (−), representing the nominal steady state, higher and lower than the nominal steady state, respectively. Branch signs + and − indicate whether values of the cause and effect variables tend to change in the same or opposite directions. A zero branch sign may be used to indicate the nonapplicability of a branch in a given context. For example, the branch between a measured variable and its sensor is not applicable if the sensor fails to a fixed value.

Derivation of the SDG is discussed in detail by Iri et al. (1979) and Palowitch (1987), and only a summary is presented here. The SDG is derived from a dynamic process model, represented as a set of algebraic, ordinary differential and partial differential equations. For differential equations with explicit time dependence, causal branches can be derived directly, as explained below. Algebraic equations that represent pseudo-steady-state approximations of dynamic equations if possible should be restored to differential equation form. Other algebraic equations have no explicit directionality and thus the causal relationships among variables cannot be unambiguously determined based solely on the structure of the equation. Knowledge of the origin of the equation, the underlying processes, device physics, and context must be utilized to determine this directionality. For example, the direction of causality between flow (F) and valve stem position (V_s) derived from the algebraic equation describing a (correctly working) control valve,

$$F - f^{+}(V_s, \Delta P) = 0 \tag{12}$$

where f^{+} is a monotonically increasing function, it is from V_s to F and not *vice versa.* To help specify digraph arcs corresponding to algebraic equations, Palowitch (1987) classifies algebraic equations into three types: driving force equations, functional relationships, and algebraic equalities. For each category, a standard set of arc specification procedures are presented.

The direction of causality between variables from ordinary differential equations,

$$d\underline{x}/dt = \underline{f}(\underline{x}, \underline{u}, \underline{p}); \quad \underline{x} = \underline{x}_0, \underline{u} = \underline{u}_0, \underline{p} = \underline{p}_0 \tag{13}$$

is from the right to the left hand side of the equation. If m is the order of the first nonzero partial derivative, $\partial^m f_i/\partial x_j^m$, evaluated at the nominal steady state of Eq. 13, the sign $[\beta_{ij}]$ of the SDG branch β_{ij} originating at x_j and ending at x_i is:

i) $[\partial^m f_i/\partial x_j^m]$, for m odd.

ii) $[\partial^m f_i/\partial x_j^m] \cdot [dx_j]$, for m even, where $[dx_j]$ is the direction of deviation of x_j from its nominal steady-state value.

Analogous rules govern branches between u_i and x_i, and p_i and x_i. Self-cycles ($i = j$) follow the same sign conventions, but are usually not depicted in the SDG. (As will be discussed later, the sign of self-cycles are required to locate variables whose ultimate response may be excluded by the SDG.) In many cases, the derivative signs can be determined unambiguously from known ordinal relationships (e.g., relative stream temperatures), and detailed numerical information is not required. When the partial derivative sign cannot be determined unambiguously from ordinal relationships, two parallel branches with opposite signs are introduced. Inequalities for determining the range of validity of the SDG are defined similarly to those for confluences.

Partial differential equations can be reduced to ordinary differential equations by the method of lines or a similar method, thus the SDG can be derived for distributed systems according to Eq. 13. In numerical simulation, many spatial discretization points may be required to provide acceptable accuracy. In qualitative simulation, relatively few discretization points are required to determine all actual qualitative system behaviors, after which further discretization does not yield additional real behaviors but may lead to generation of spurious solutions (Palowitch, 1987). The optimum discretization is determined by trial and error.

Determining system behavior from the SDG

In simulating the effect of malfunctions on a process, it is assumed that the process is at steady state prior to fault initiation, so all nodes initially have the value 0. The immediate effect of a malfunction is to cause a deviation of a single process variable, input or parameter (the root node) from its initial value. The deviation of the root node (the primary deviation) is the source of all subsequent disturbances, determined by propagating the disturbance from the root node to other nodes under a fixed set of simulation assumptions. Ideally, simulation assumptions should be chosen so that the interpretations include the complete set of actual behaviors for all members of the system's qualitative class (completeness) and as few spurious behaviors as possible (minimality). Within the hypothesis/test diagnostic framework, completeness is crucial as it guarantees the inclusion of the failure origin, while minimality is desirable because it leads to improved diagnostic resolution.

The following are some of the useful definitions:

- A path from an initial to a terminal node is a directed sequence of nodes and branches in the SDG or ESDG.
- An acyclic path is a path where all nodes (including initial and terminal) appear only once.
- A loop is a path that has the same initial and terminal nodes, where each branch is traversed only once.
- An event is any change of node sign.
- The influence of a node x_j on node x_i is the product $[\beta_{ij}] \cdot [dx_j]$.
- The net influence of a set of nodes x_j on a node x_i is the qualitative sum of the individual influences, $\Sigma_j [\beta_{ij}] \cdot [dx_j]$.
- The initial response is defined as the first nonzero sign assumed by each node. There may be more than one possible initial response.
- The ultimate or steady-state response is any reachable state where each node with an unambiguous net influence has the same sign as the influence. There may be multiple possible ultimate responses.

The following two rules serve to generate sequences of events locally consistent with causality:

Rule 1. Any node can change its sign provided that the new sign equals the net influence on the node. (Note that the ambiguous influence, ?, matches any node sign.)

Rule 2. Direct transitions from (+) to (−) and (−) to (+) are forbidden. These rules imply that, if an event occurs at x_i, the sign change will be in the direction of a nonzero input influence or, if all influences are zero, x_i can return only to normal. Expressed mathematically, when node x_i undergoes a sign change:

$$([dx_i]_k - [dx_i]_{k-1}) \cdot [\beta_{ij}] \cdot [dx_j] = (+), \text{ for some } j,$$

$$\text{or} \quad [dx_i]_k = 0 \text{ and } [\beta_{im}] \cdot [dx_m] = 0, \text{ for all } m, \quad (14)$$

where $[dx_i]_{k-1}$ is the old node sign and $[dx_i]_k$ is the new node sign. The influences consistent with the direction of change of x_i are the possible causes of the event, that is, any node x_j input to x_i for which Eq. 14 is satisfied.

The interpretations generated by Eq. 14 will include all cases of inverse and compensatory response associated with feedback loops (Oyeleye, 1988). Since inverse and compensatory responses are exhibited by relatively few process systems outside of control loops, Rules 1 and 2 can lead to many spurious interpretations. [The multistage signed directed graph (Umeda et al., 1980) gives the same results as interpreting the SDG under Rules 1 and 2).] For example, high temperature $[dT] = (+)$ on the shell side of a heat exchanger will cause increased rate of heat flow to the tube side, $[dQ] = (+)$. Causally, $[dQ] = (+)$ has a negative influence on T. According to Eq. 14, transitions to the states $[dT] = (0)$ and subsequently $[dT] = (-)$ are permissible; however, these behaviors would not be observed. To limit the production of spurious interpretations associated with feedback effects, we adopt an additional assumption regarding the behavior of feedback loops. Put loosely, this assumption is that "an effect cannot compensate for its own cause." Thus, $[dQ] = (+)$, the effect, would not be allowed to override the cause, $[dT] = (+)$. More formally, using the definition of causality associated with Eq. 14, a causal path can be defined as an ordered list of events beginning with the primary deviation, where each event causes the next event in the list. A simple causal path (SCP) can be traced from the primary deviation to any subsequent event without repeating a node. Therefore, SCP's can be mapped onto acyclic paths in the SDG. The heuristic, "an event cannot compensate for its own cause," can be implemented by limiting disturbance propagation to SCP's:

Rule 3. A node is permitted to change its sign only if there is a simple causal path between the new event and the primary deviation. In the previous example, the causal path $[dT] = (+) \rightarrow [dQ] = (+) \rightarrow [dT] = (0)$ is not simple because the node T is repeated. A major reduction of spurious solutions is achieved through the SCP assumption; however, further measures are required to guarantee completeness.

Limitation of the simple causal path assumption

Generally efficacious, Rule 3 leads to exclusion of certain realizable responses when compensatory or inverse responses actually do occur. Compensatory responses occur by design in control loops and therefore previous authors have devised special rules for interpreting the qualitative behavior of control loops. For example, in their diagnostic algorithm, Iri et al. (1979) permit compensatory response for controlled variables in feedback loops, but otherwise require SCP's. However, the approach of devising a set of special exceptions to Rules 1–3 is not satisfactory. For example, the response predicted by Rules 1–3 to a slow partial blockage in the outlet pipe of the tank shown in Figure 2a

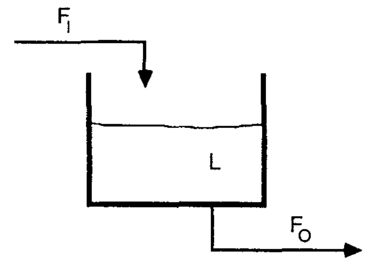


Figure 2a. Schematic of tank.

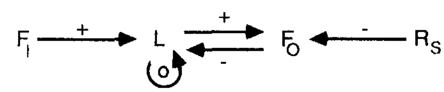


Figure 2b. SDG of tank.

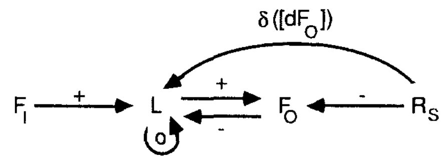


Figure 2c. ESDG of tank.

(increase in resistance R_s in Figure 2b) is that the level increases while the outlet flow decreases. However, the outlet flow exhibits compensatory response and ultimately returns to the initial value (0). Because this compensatory response is not due to the action of controllers, Iri's method and its relatives (Shiozaki et al., 1985; Tsuge et al., 1985b) fail to diagnose this malfunction correctly if the negative deviation of outlet flow is sufficiently small (blockage sufficiently slow), despite the fact that latter methods use a five-range pattern. Presented are the rigorous conditions under which the SCP assumption fails.

Oyeleye (1988) shows that propagating the effects of disturbances using the simple causal path assumption is guaranteed to provide the initial response of the system. Thus, interpretations of the SDG may exclude the ultimate response of a system only in situations where a variable exhibits inverse (IR) or compensatory response (CR). IR and CR are the net result of opposing causal effects that arise from: i) multiple acyclic (feedforward) paths to a node; ii) negative feedback control loops; or iii) other negative feedback loops. Rules 1–3 account for IR and CR arising from i) and ii). However, in cases where IR and CR arise from feedback effects in noncontrol loops (or when CR is caused by disturbances entering control loops at variables other than control variables), the simulation rules fail.

Inverse variables (IV's) and compensatory variables (CV's) are defined as variables that exhibit IR or CR to a particular disturbance due to negative feedback. IV's can always display CR by varying parameter values within $\underline{C}$. We restrict CV's to be variables that do not exhibit IR for any numerical realization of the qualitative class. We make the following additional definitions:

- A cycle is a loop in the SDG, in which the initial and terminal nodes are the same and all other nodes in the loop are traversed only once.
- The complementary subsystem to an acyclic path in the SDG is the subgraph that is obtained if all nodes in the acyclic path (including initial and terminal nodes) are eliminated.

• The complementary subsystem to a cycle in a subgraph of the SDG is the subgraph obtained if all nodes in the cycle are eliminated from the original subgraph.

• A strongly connected component (SCC) of the SDG is a subgraph of the SDG for which a path exists from every node u to every node v (and from v to u) in the SCC; and the SCC is not a proper subgraph of any other SCC (Tarjan, 1972).

• A disturbance node to a SCC is an adjacent node, not located in the SCC from which at least one branch exists to a variable in the SCC.

The authors have derived necessary conditions for locating variables (IV's and CV's) whose ultimate values may be excluded by the SDG when using the SCP assumption. (Proof of these conditions is presented in the supplementary material.) These conditions are derived using stability constraints and are related to the topology and signs of self-cycles of the SDG. In order to identify IV's and CV's with respect to perturbations in inputs, it is sufficient to consider the response of variables in SCC's with respect to perturbations in their respective disturbance variables. For stable systems, the necessary conditions for a variable in a SCC to display IR due to negative feedback to perturbations in a disturbance variable are:

1) The IV is located in a negative feedback loop or cycle (except self-cycles).

2) The complementary subsystem to one of the acyclic paths from the disturbance variable to the IV should contain a positive cycle (or self-cycle).

3) The complementary subsystem to the positive cycle in one of the complementary subsystems in 2) should violate either (5a, 5b or 6) below.

Similarly, for stable systems, the recursive necessary and sufficient conditions for a variable in a SCC to display CR due to negative feedback to perturbations in a disturbance variable are:

4) The CV is located in a negative feedback loop or cycle (except self-cycles).

5) The complementary subsystems to all acyclic paths from the disturbance variable to the CV should each: a) have at least one zero self-cycle (integrator); and b) do not have a cycle containing all variables in the subsystem.

6) The complementary subsystems to all nonzero cycles (excluding self-cycles) in each complementary subsystem in 5) should each satisfy (5a, 5b and 6).

Necessary conditions (Eqs. 1–3) for IR result in a potential set of IV's with respect to perturbations in a disturbance variable. For a particular system, the actual set of IV's could be any of the subsets of this set. Some of these subsets can be eliminated if the sign of all acyclic paths from the disturbance variable to each variable in the SCC in unique. A subset of possible IV's is consistent only if the sign of the net influence (using ultimate values) on each variable in the SCC is either ambiguous or opposite to the product of the sign of the variables ultimate value and its self-cycle:

$$\sum_j [\beta_{ij}] \cdot [dx_j] = - [\partial f_i/\partial x_i] \cdot [dx_i]; \qquad i = 1, 2, \ldots n \text{ (steady state)} \quad (15)$$

Applying these conditions to the tank (Figure 2a), the SCC's of the SDG are (L F_0), (F_1) and (R_s). Of the SCC's only (L F_0) contain variables in a negative feedback loop. The complementary subsystem to the acyclic path from disturbance variable R_s to F_0 is (L). There is a zero self-cycle on L, as level exhibits integrating effects. Within this subsystem, no nonzero cycles exist and thus F_0 is a CV with respect to R_s. The criteria correctly predicts the ultimate response of the system for outlet blockage.

One can also show that CR of controlled variables in feedback control loops is a special case of the more general behavior of CV's in negative feedback loops. Figure 3a shows the SDG of a feedback control loop with PI control. X, X_c, X_m, X_s, X_v, and X_{sp} are the controlled variable, controller output, manipulated variable, controlled variable sensor, valve position, and set point, respectively. Y_i represent other nodes outside the loop. The SCC of interest is (X, X_s, X_c, X_v and X_m) and all variables in the SCC are in a negative feedback loop, thus satisfying Eq. 4. The controller output node, X_c is associated with integral action and has a zero self-cycle. The disturbance variables to the SCC are Y_i and X_{sp}.

With respect to a perturbation in Y_3, there is only one acyclic path to each of the variables in the loop. The complementary subsystems to the acyclic paths from Y_3 to each of X_m, X, X_s, X_c, and X_v are subsystems (X, X_s, X_c, X_v), (X_s, X_c, X_v), (X_c, X_v), (X_v) and ϕ (ϕ is the null system), respectively. Subsystems (X, X_s, X_c, X_v), (X_s, X_c, X_v) and (X_c, X_v) each contain X_c (Eq. 5a). In addition, none of these subsystems contains a nonzero cycle (Eqs. 5b and 6). Thus, X_m, X, X_s are all compensatory variables with respect to Y_3. Note that, in this situation, where the disturbance enters the loop through the manipulated variable, the correct process behavior provided by the above analysis is not accounted for by the SDG nor by previous "special rules" for control loops. The analysis also predicts that both X and X_s are compensatory variables with respect to perturbations in each of Y_1 and Y_2 and that there are no compensatory variables with respect to set point changes (X_{sp}).

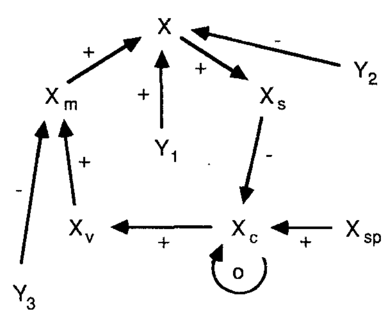


Figure 3a. SDG of feedback control system.

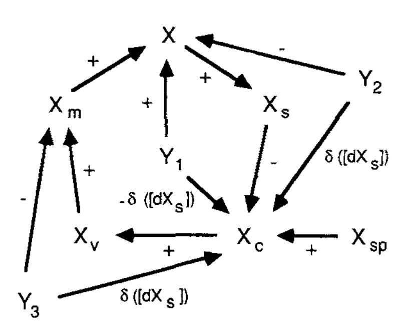


Figure 3b. ESDG of feedback control system.

Extended signed directed graph

In the previous section, cases when interpretations obtained from the SDG (using the SCP assumption) may exclude the ultimate response of the system from stable steady states were identified. In this section, the SDG is modified to the extended signed directed graph (ESDG). The ESDG contains all nodes and branches in the SDG and in addition, contains certain nonphysical feedforward paths (branches) that explain IR and CR in negative feedback loops. The ESDG is constructed so that simulation can be conducted under the SCP assumption without exceptions for control loops. The ESDG is guaranteed to produce interpretations which include the ultimate system response from stable steady states for all realizations of system parameters within the scope of its qualitative class.

ESDG Branches for IR. Deriving the IR branches of the ESDG involves identifying IV's on each acyclic path from the disturbance variables based on the criteria described earlier. On these acyclic paths, the IV's occur as one or more strings of adjacent variables. For each string of IV's on an acyclic path, ESDG branches for IR originate at the node just upstream of the IV's and terminate at the noninverse SCC variable located just downstream of the string. The sign of the branch is the product of the signs of the branches on the forward path in the SDG between the origin and termination of the ESDG branch. In effect, the ESDG branches "jump over" the IV's providing a SCP accounting for IR.

ESDG Branches for CR. The topology of ESDG branches accounting for CR due to negative feedback is the same as for IR branches. However, to prevent prediction of IR by the CV's, we assign to the ESDG branches the sign $\pm\delta([dx_j])$, where δ is the "qualitative Dirac delta function," Table 1, and x_j is the CV located just upstream of the termination of the ESDG branch. Only when $[dx_j]$ is zero does the ESDG branch come into play, allowing the disturbance to "jump" over the CV's.

Considering the gravity flow tank, F_0 is a CV with respect to R_s on the only acyclic path from R_s. Thus, one ESDG branch with sign $+\delta([dF_0])$ from R_s to L (the noncompensatory variable) is required, Figure 2c. The positive sign associated with the δ function reflects the net sign of the path from R_s to L in the SDG. This branch enables the correct ultimate behavior of the system to be predicted using the SCP assumption. Similarly, three ESDG branches, Figure 3b, are required for the example with the control loop, all terminating at X_c. A branch with sign $-\delta([dX_s])$ from Y_1, one with sign $+\delta([dX_s])$ from Y_2 and another with sign $+\delta([dX_s])$ from Y_3.

In conclusion, special treatment is not required for disturbance propagation in control loops when using the ESDG for qualitative simulation. After ESDG branches are added to the SDG, disturbances can be assumed to propagate along SCP's only.

Deriving steady-state constraints from the ESDG

We showed previously how confluences derived from noncausal sources constrained the ultimate behavior of the system. The ESDG, presented initially as a graph, can also be represented as an equivalent set of confluences. Conversion of the ESDG to confluences provides a convenient uniform representation for both causal and noncausal constraints. In this section, we show how a set of confluences can be derived from the ESDG. The confluences derive from two sources: from local balances around nodes of the ESDG and from the global topology of the ESDG relating to positive feedback loops.

Nodal Balances. The definition of ultimate response presented earlier implies that, at a steady state, the sign on each ESDG node (except the primary deviation) must equal the net influence on the node:

$$[dx_i] = \sum_j [\beta_{ij}] \cdot [dx_j] \quad \text{(steady state)} \tag{16}$$

We refer to these constraints as "nodal balances."

Restriction to SCP's. Although a given pattern of node signs may be consistent with the nodal balances, it may not be feasible to produce such a pattern by propagation on simple causal paths from the given initial conditions. Any causal path associated with acyclic paths in the ESDG must be a simple causal path. Thus, the only possible sources of complex causal paths are feedback loops in the ESDG.

In a negative feedback loop, in general, invoking a complex causal path results in violation of at least one nodal balance at steady state. Specifically, invoking a complex causal path results in IR (or CR), and there will be an inconsistency in the nodal balance for the noninverse (noncompensatory) loop variable just downstream of the inverse (compensatory) loop variables. Thus, Eq. 16 is sufficient to eliminate behaviors associated with complex causal paths in systems with negative feedback loops.

Such is not the case in systems with positive feedback loops. Consider the ESDG of the system with a positive feedback loop shown in Figure 4. The nodal balances on x_1 and x_2 are:

$$[dx_1] = [dx_2] + [du]$$
$$[dx_2] = [dx_1] + [du] \tag{17}$$

If $[du] = (+)$ or (0), Eqs. 17 have a solution $[dx_1] = [dx_2] = (-)$, which is clearly inconsistent with the ESDG under the SCP assumption. These interpretations are due to a causal loop in which the cause of $[dx_1] = (-)$ is $[dx_2] = (-)$, and *vice versa*, unsupported by an external cause. For asymptotically stable physical systems, disturbances in feedback loops cannot persist as a sustained input is required to maintain an output (Bode stability requirement). In order to remove the spurious behavior, an additional confluence that forces at least one node in the loop to assume the sign of an external influence is required. Eq. 18a

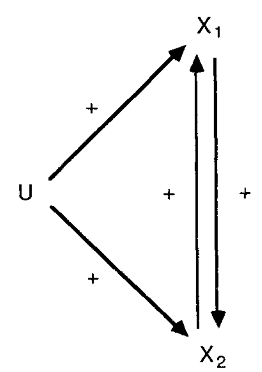


Figure 4. ESDG of system with positive feedback loop.

achieves the desired effect:

$$[dx_1] = [dx_0] \text{ or } [dx_2] = [dx_0] \quad (18a)$$

Disjunction of confluences presents some computational difficulties, and it is more convenient to replace Eq. 18a with the equivalent representation:

$$\delta([dx_1] - [dx_0]) + \delta([dx_2] - [dx_0]) = (+) \quad (18b)$$

In general, an additional confluence is required for each positive feedback loop that may be isolated from the disturbance origin. These confluences are of the form,

$$\delta([dx_{j1}] - [\beta_{j1}] \cdot [dx_{i1}]) + \ldots + \delta([dx_{jn}] - [\beta_{jn}] \cdot [dx_{in}]) = (+) \quad (19)$$

where x_{ik} ($k = 1, 2, \ldots n$) are disturbance variables to nodes x_{jk} within the loop. The confluences in Eqs. 16 and 19, combined with the confluence representing the primary deviation(s), provide necessary and sufficient conditions for steady state consistency with the ESDG.

Constraints derived from causality

The ESDG provides two types of constraints important in eliminating spurious interpretations in steady state modeling. First, the ESDG provides constraints that are latent in the independent steady-state equation set, but may be difficult to derive by algebraic manipulation. Second, stability criteria are used in deriving the ESDG, and thus a set of "nonlatent" confluences that may eliminate some interpretations associated with the response from unstable steady states are provided. The latter are important because the set of basic and latent confluences derived from steady state equations produces the response from all stable and unstable steady states. The following two examples demonstrate the utility of the latent constraints derived from the ESDG.

Example 1: Latent Confluences from ESDG. An important latent constraint in modeling countercurrent heat exchangers involves the hot fluid outlet temperature:

$$[dT_{HO}] = [dT_{HI}] + [dT_{CI}] + [dF_H] - [dF_C] - [dU] \quad (20)$$

Beginning with the basic heat balances, several complex steps involving partial solution, substitution, and simplification are required to arrive at Eq. 20. In addition, it is difficult to determine the signs of the partial derivatives associated with each term in Eq. 20 for all numerical realizations of parameter values. Although it is difficult to derive this relationship analytically, this confluence results directly from a nodal balance around T_{HO} in the ESDG of the heat exchanger.

Example 2: Nonlatent Confluences from ESDG. Consider the isothermal, irreversible, autocatalytic reaction $A \rightarrow B$, first order in A and second order in B, taking place in a continuous stirred tank reactor (CSTR) with constant space velocity. The dynamic process equations are:

$$\frac{dC_A}{dt} = \frac{F(C_{AO} - C_A)}{V} - k_r C_A C_B^2 \quad (21a)$$

$$\frac{dC_B}{dt} = k_r C_A C_B^2 - \frac{FC_B}{V} \quad (21b)$$

The corresponding noncausal, steady-state confluences are:

$$[dC_{AO}] = [dC_A] + [dC_B] \quad (22a)$$

$$[dC_A] + [dC_B] = 0 \quad (22b)$$

Table 3 lists the solutions to these confluences for an increase in reactant feed concentration. These solutions correspond to the response from the two steady-state solutions of Eqs. 21, for $C_{AO}^2 > 4F/k_rV$:

$$C_{AS} = \frac{C_{AO}}{2} \mp \frac{(C_{AO}^2 - 4F/k_rV)^{1/2}}{2} \quad (23)$$

The latter solution in Table 3 (invoking the plus sign in Eq. 23) corresponds to the unstable steady state.

The ESDG for this system is shown is Figure 5. The branch between C_{AO} accounts for possible inverse response of C_A to changes in C_{AO}, derived by the previous criteria. Nodal balances yield the following confluences:

$$[dC_A] = [dC_{AO}] - [dC_B] \quad (24a)$$

$$[dC_B] = [dC_A] + [dC_{AO}] \quad (24b)$$

The first of these is the same as Eq. 22a, however, Eq. 24b is a new nonlatent constraint which eliminates the response from the unstable steady state. Thus, the response from the stable steady state is the only one that satisfies both the noncausal confluences and the ESDG.

Qualitative Simulation of a Reactor System

To demonstrate the use of combining causal and noncausal constraints in determining steady-state qualitative behavior of processes, we consider the process shown in Figure 6. In this process, an irreversible heterogeneous catalytic exothermic reaction ($A \rightarrow mB$) with rate expression

$$r_A = k_r C_A^n, n > 0 \quad (25)$$

takes place in a continuous stirred tank reactor. To provide temperature control, part of the reactor outlet stream is recycled to the reactor through a heat exchanger. The recycle flow rate is controlled, and residence time in the reactor is controlled by maintaining the level of reactants in the reactor. Constant boundary pressures of all input and output streams and constant physical properties are assumed. The objective is to determine the ultimate qualitative response of the system to various faults and disturbances.

The process provides several interesting interactions between

Table 3. Solutions to Confluences of Autocatalytic Reaction

Solution	C_{AO}	C_A	C_B
1	+	−	+
2	+	+	−

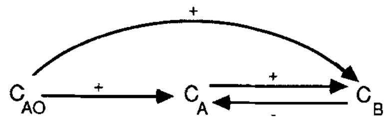


Figure 5. ESDG for autocatalytic reaction in Example 2.

its control loops, and its ESDG has many multiple causal pathways with net opposing signs, tending to generate a great deal of ambiguity when subjected to qualitative analysis. The system is nonlinear and can attain multiple steady states (some unstable) in the absence of temperature control. Thus, it is a challenging example for qualitative modeling.

The process ESDG, causal confluences and details of derivation of noncausal confluences are provided as supplementary material and only aspects pertinent to the following discussion are presented. The inequalities defining the scope of the validity of the confluences (all variable and parameter values are assumed to be positive) are that:

i) Reactor outlet flow rate (F) is greater than the recycle flow rate (F_R).

ii) Reactor temperature (T) is higher than the recycle temperature (T_R).

iii) Pressure drop in each of the conduits is positive.

These conditions are violated only in cases of reverse flow in the product, recycle or cooling streams, or the cooling system acting as a heat source (due to either an external heat source or the cooling water inlet temperature being higher than the reactor temperature). For most malfunctions, transitions between qualitative regimes, due to violation of these conditions, will not occur.

Depending on fault magnitudes, perfect control of controlled variables may be maintained or control loops may become saturated at the new steady state. Control loop saturation will be allowed and confluences describing controller behavior account for these transitions. This is done by forming a disjunction of confluences relating to perfect control and controller saturation. The only other transitions that may occur are to regimes where process equations are no longer valid, such as boiling. Therefore, it is not very limiting to assume no transitions (as described previously) except for control loop saturation.

A representative set of malfunctions for this system are listed in Table 4. Malfunctions and disturbances are introduced by a qualitative change in one or more process inputs or parameters,

Table 4. Selected Malfunctions for CSTR with Recycle

	Malfunction
1	normal operation
2	pipe 1 partially blocked
3	pipe 6 partially blocked
4	feed concentration high
5	recycle flow set point high
6	fouled heat exchanger
7	deactivated catalyst
8	temp control valve stuck high
9	leak in reactor
10	recycle flowmeter stuck high

or by modifying the appropriate confluences. (Although system response in multiple fault situations is not presented, multiple faults can be modeled by modifying all relevant confluences for individual faults in the multiple fault set.) The first four columns of Table 5 show the number of qualitative steady-state solutions for the set of 14 measured variables (controller outputs also measured) when using:

i) Confluences derived from the ESDG.

ii) Confluences derived from an independent "basic" set of 27 equations in 27 unknowns.

iii) Combination of confluences from i) and ii).

iv) Confluences in iii) with 24 additional latent confluences derived from the independent equation set.

Table 5. Number of Valid Solutions Obtained by Utilizing Confluences from Various Sources

Fault	Casual (ESDG) (i)	Local (Noncausal) (ii)	Causal & Local (iii)	Causal, Local & Latent (iv)	Causal, Local, Latent & Functional (v)
1	1	279	1	1	1
2	107	984	481	141	3
3	501	1,359	192	13	1
4	12	287	10	10	1
5	501	4,869	192	13	1
6	2	279	2	2	1
7	4	281	4	3	1
8	1	279	1	1	1
9	984	1,080	178	35	1
10	309	1,215	138	9	1

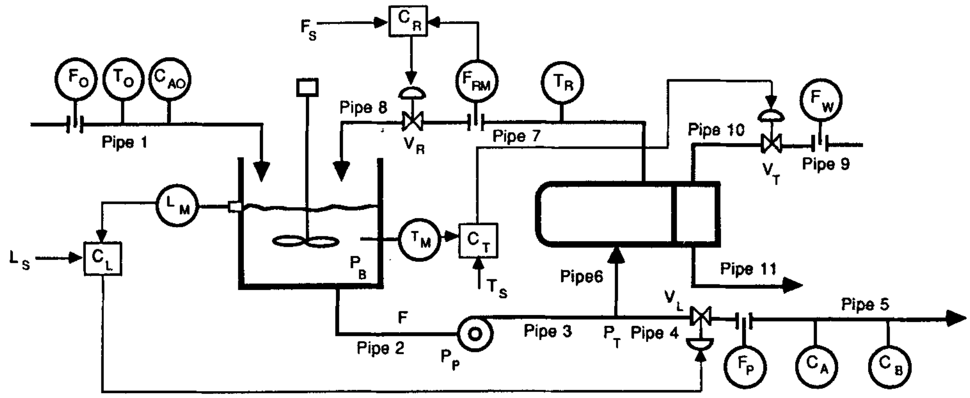
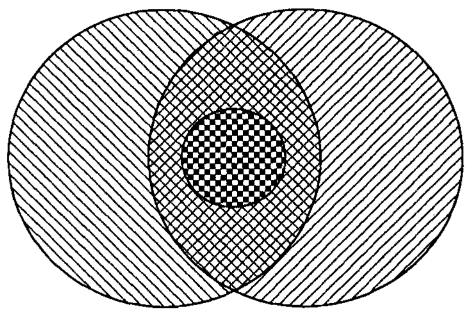


Figure 6. Continuous stirred tank reactor with recycle.



causal confluences from ESDG (case i)

local non-causal confluences (case ii)

causal and local non-causal confluences (case iii)

causal, local and latent non-causal confluences (case iv)

Figure 7. Relationship between solutions using different sets of confluences (refer to Table 5).

The relationship between the solutions i)–iv) is most clearly seen using the diagram of Figure 7. The solutions of i) and ii) are partially disjointed, the intersection satisfying both causality and noncausal confluences iii). Addition of latent constraints derived from the independent equation set iv), further reduces the size of this solution space.

The selection of a set of independent equations for ii) and iii) is arbitrary since any 27 independent equations selected from the set of redundant equations suffices. To select the independent equations used in this example, locality was used as a criterion: that is, all equations relate to just one unit in the process. Case ii), therefore, represents the performance of a hypothetical "modular" steady-state qualitative simulator, in the absence of causal information. Combining causal and basic noncausal constraints reduces the number of solutions obtained with the ESDG by up to a factor of 2 to 3. Adding latent constraints derived from the independent equation set leads to further reductions of up to an order of magnitude. The overall reduction in the number of solutions obtained between cases i) and iv) is by up to a factor of 35, and between cases ii) and iv) by up to a factor of 370.

Using knowledge about functioning control loops to reduce ambiguity

The function of an engineering system is the purpose for which it was designed. When the systems intended function is achieved, *a priori* knowledge about the system's function can be used to reduce the ambiguity in qualitative modeling (de Kleer, 1984). In chemical process systems, feedback control loops attempt to maintain values of important variables within acceptable ranges, thus playing an important role in determining system behavior. Generally, intended function may not be achieved in malfunctioning systems, however, control loops are designed to achieve their intended function in the presence of most expected faults and disturbances. Thus, in many situations, zero deviation of the controlled variable is maintained after all transients have died out. Exceptions occur when the disturbance magnitude is large enough to cause loop saturation, or when the fault prevents loop operation, as in the case where an element of the control loop is stuck at a fixed position (zero-gain events).

Multiple solutions that arise on applying the causal, basic and latent noncausal confluences (case iv above) are the conjunction of the cases of control loop saturation and zero steady-state offset of controlled variables. The results of applying these confluences with additional constraints of zero steady-state offset (except for zero-gain events) are shown in the fifth column of Table 5. From Table 5, it can be seen that the confluences produce one solution for most faults. In cases where one solution is predicted, the solution represents the actual behavior of the system. When multiple solutions are predicted, further (analytic or possibly quantitative) analysis is required to determine the realizability of each solution. For this example, further analytic analysis of the fault producing multiple solutions (Fault 2) indicates that all three solutions are realizable.

Discussion

In this paper, it was shown that limiting disturbance propagation to simple causal paths of the SDG leads to the exclusion of the ultimate response for systems in which variables exhibit IR or CR due to negative feedback. Consequently, previous SDG based algorithms using this assumption may fail to produce the correct diagnosis. Rigorous topological conditions under which the SCP assumption fails were derived. Specifically, IR is caused by positive feedback effects inside negative feedback loops, and CR is caused by integral effects associated with negative feedback loops. On this basis, an alternative causal model of the process, the extended signed directed graph was developed. The ESDG is guaranteed to provide the full set of ultimate process responses, provided the system does not undergo transitions to other qualitative regimes. A procedure for representing the ESDG as a set of steady state constraints was also derived.

It was also shown that noncausal local and latent constraints and causal latent and nonlatent constraints are necessary in order to determine the final qualitative response of continuous processes to faults and disturbances. Although qualitative methods inherently lead to ambiguous interpretation of a system's behavior, combining these sources of constraint information leads to a substantial reduction in the number of spurious interpretations of a system's behavior. If an analytical steady state solution to the system exists, the set of independent and latent constraints can theoretically eliminate all spurious solutions except unstable steady states, which are addressed by nonlatent constraints derived from the ESDG. However, because of analytical complexities in deriving latent contraints and because the nonlatent constraints from the ESDG are not sufficient conditions on the removal of all unstable steady states, there is no guarantee that the method presented will eliminate all spurious solutions. A set of heuristics that have proven useful in deriving latent constraints have been reported. In the example considered, combining sources of constraints reduced the number of interpretations obtained by using local noncausal constraints and causal constraints by up to two orders of magnitude.

These constraints do not express knowledge about a system's function, which may be useful in resolving ambiguity when the intended function is achieved. Ambiguity was further reduced by applying *a priori* knowledge about functioning control loops. All spurious solutions were eliminated in examples where additional constraints of functioning control loops were applicable.

There are some other limitations in applying the steady state patterns obtained from using the steady state causal and noncausal confluences. Dynamic effects were ignored, and it was assumed that the same confluences are also applicable at the new steady state. This assumption is violated when transitions to different qualitative regimes occur, and could lead to exclusion of the correct steady state solution. This method is not applicable to predictive safety analysis, where qualitative transitions are of primary importance. In processes that exhibit inverse response, compensatory response or display oscillatory behavior, the steady state patterns may also exclude some transient patterns. This is important in systems with large time constants where the system takes a "long" time to achieve a new steady state. A richer representation of the behavior of equipment and process streams is required to incorporate these dynamic effects.

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Notation

A, B = chemical species, A, B
C_A, C_B = concentration of A, B in reactor
C_{AO} = feed concentration of A
C_L, C_R, C_T = controller output signals
f^+, f^- = strictly monotonic increasing, decreasing functions
F = volumetric flowrate
F, F_O, F_p = reactor outlet, feed, product flow rates
F_R, F_{RM}, F_S = recycle flow rate, measurement, setpoint
F_W = cooling water flow rate
k_r = reaction rate constant
L = reactor, tank level
L_M, L_S = reactor level measurement and setpoint
m = stoichiometric coefficient
n = order of reaction
p = process parameter
P_1, P_2, P_T = nodal pressures
P_B = reactor base pressure
P_p = pump head
Q = heat flowrate
r_A = reaction rate
R_s = flow resistance in conduit
t = time
T, T_O, T_R = reactor, feed, recycle stream temperatures
T_M, T_S = reactor temperature measurement, setpoint
T_{WI}, T_{WO} = cooling water inlet, outlet temperatures
u = input variable
U = heat transfer coefficient
V_L, V_R, V_T = control valve stem positions
V_s = valve stem position
x = system state variables

Greek letters

β = branch in SDG or ESDG
δ = qualitative Dirac delta function
ϕ = null system
ΔH_R = heat of reaction
ΔP = pressure drop
[ ] = sign of expression
| | = absolute value of expression
$\cdot$ = qualitative multiplication

Subscripts

c = controller output signal
C = cold stream
H = hot stream
I = inlet
$i, j, k, \ldots$ = dummy variables
O = outlet
m = manipulated variable
s = sensor value
S = steady-state value
sp = controlled variable set point
v = control valve

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