Comparative Analysis of Qualitative Models When the Model Changes

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An important application of the recently developed techniques in qualitative mathematical modeling is to qualitatively predict how changes in the operation of chemical units affect their behavior. Weld (1987, 1988a,b) has developed a series of comparative techniques that analyze the effect of perturbations to the parameters of a given qualitative unit model. In this article we demonstrate a system, based on the qualitative process theory of Forbus (1984), which extends comparative analysis in two ways. First, it predicts the effects of changes in the qualitative equations and in parameter values. Secondly, it compares physical descriptions, rather than comparing models directly, and builds and compares the associated models automatically.

Introduction

Reasoning with qualitative models of process units is an important component of intelligent systems which reason with "deep" or "first principles" knowledge of chemical plants (Dalle Molle et al., 1988; Oyeleye and Kramer, 1988; Rich and Venkatasubramanian, 1987). Comparative analysis is a branch of qualitative reasoning that predicts how changes to the inputs of a unit model affect the behavior of model parameters. It can be viewed as the qualitative analog of sensitivity or perturbation analysis of a set of equations. Comparative analysis is required for many intelligent systems. For example, in "generate and test" troubleshooting systems it is necessary to determine how hypothesized faults would change the behavior of process units (Grantham and Ungar, 1990), and in design it is necessary to compare the relative effect on process behavior of alternative design scenarios (Grantham, 1990).

Comparative analysis systems demonstrated to date are limited to analyzing the effect of changes to parameter values; the actual qualitative constraints that define the structure of the model must remain constant. Thus, although these systems can predict that an increase in the input temperature to a liquid preheater results in a higher output temperature they cannot predict that some of the liquid may vaporize. Neither can they predict that the addition of catalyst to the input would result in an exothermic reaction which would increase the exit temperature of the liquid and change its composition.

To make such deductions, comparative analysis systems must be extended in two ways. First, they must recognize that changes in a physical description may result in a change in the structure of the qualitative model, i.e., they must take on the task of modifying a model to reflect changes in process conditions rather than requiring it to be specified *a priori*. Secondly, they must be able to compare the modified and original models to determine how the structural changes affect behavior. It is, of course, still necessary to be able to analyze parameter changes within a single model.

A comparative analysis system is presented here which combines automatic model modification with model-model comparison. This enables the system to automatically determine the effects of changes in process conditions, which change the appropriate model for process units.

Background

Several techniques have been presented that qualitatively predict how perturbations to process parameters affect the behavior of steady-state qualitative models of chemical engineering systems. For example, given a qualitative model of a heat exchanger they could predict how changes to the input temperatures, heat transfer coefficient, or fluid flow rates would affect the output temperatures. These include causal constraints (D'Ambrosio, 1989), signed digraphs (Iri et al., 1979; Umeda et al., 1980; Oyeleye and Kramer, 1988), and confluence models (Rich and Venkatasubramanian, 1987; Oyeleye and Kramer, 1988). These systems are limited in that they only consider steady-state behaviors, do not consider transitions into new qualitative states, and assume that the parameter

Changes to the qualitative model arise when the process conditions are modified such that the physics or chemistry underlying the behavior is changed. This may occur in two circumstances: either when a new object is introduced into the process description (for example, addition of catalyst to a heat exchanger stream) or when a parameter makes a transition to a new qualitative value (for example, the liquid stream of a heat exchanger unexpectedly reaching its boiling point before reaching the exit).

The system comprises the following components, which will be considered in detail in the following sections:

- Mapping from changes in process conditions to changes in the model
- Comparing modified and original models
- Predicting the resultant changes in behavior (i.e., relative changes at each transition, changes to interval durations, and changes in transitions).

Behavior which consists of a single qualitative state will be presented first. We will then show how this can be extended to behavior which is described by a sequence of qualitative states.

Terminology

Following the terminology of Kuipers (1986), the qualitative behavior of any system is defined by the values of each variable and its derivative at and between an ordered sequence of distinguished time points (T_i). A distinguished time point is an instant at which some variable (or its derivative) changes qualitative values. For example, the vaporizer described in the previous section is described by three distinguished time points corresponding to the time of entrance to the pipe (distance = 0), time at which vaporization first occurs (temperature = boiling point) and the time of exit from the pipe (distance = pipe length). The behavior of a variable, q, at any time point, T_i, is described in terms of a qualitative value, $QS(q, T_i)$, and the sign of its derivative, $QDIR(q, T_i)$. Similarly, the behavior of a variable over the interval between two distinguished time points, T_i and T_{i+1}, is described by a value, $QS(q, T_i, T_{i+1})$, and a derivative, $QDIR(q, T_i, T_{i+1})$.

For example, the behavior of the temperature of an elemental volume of fluid as it passes through the vaporizer is described as follows:

Time Point/Interval	QDIR Temp.	QS Temp.
T_0 (distance = 0)	+	0 < Temp. < boiling pt.
$[T_0, T_1]$	+	0 < Temp. < boiling pt.
T_1	0	Temp. = boiling pt.
$[T_1, T_2]$	0	Temp. = boiling pt.
T_2 (distance = pipe-length)	0	Temp. = boiling pt.

Modifying the terminology of Weld (1988), changes in the qualitative behavior of variables are defined in terms of relative changes. For example, $RC\text{-}QDIR(q, T_i, T_{i+1}) = +$ indicates that the derivative of q over the interval $[T_i, T_{i+1}]$ has increased, i.e., it has experienced a positive relative change. Similarly, $RC\text{-}QS(q, T_i) = 0$ indicates that the value of q at time point T_i has not changed.

Let us also define the duration of an interval $[T_i, T_{i+1}]$, i.e., the time between the two consecutive time points, as $DUR(T_i, T_{i+1})$ and the relative change in duration as $RC\text{-}DUR(T_i, T_{i+1})$.

```
(Reaction ?11)
    Individuals:          ?11 a 2 component liquid of form (2-c-l-p A B ?c)
    Preconditions:        (contains ?c catalyst)
    QuantityConditions:   (greater-than (mf A ?11) (m-equil-mf A ?11))
    Relations:            (Qprop reaction-rate (temperature ?c))
                          (Qprop reaction-rate (mf A ?11))
                          (Qprop- reaction-rate (m-equil-mf A ?11))
    Influences:           (I+ (heat ?c) reaction-rate)
                          (I+ (amount-of B ?11) reaction-rate)
                          (I- (amount-of A ?11) reaction-rate)
```

Figure 2a. Simplified description of the phenomenon "reaction".

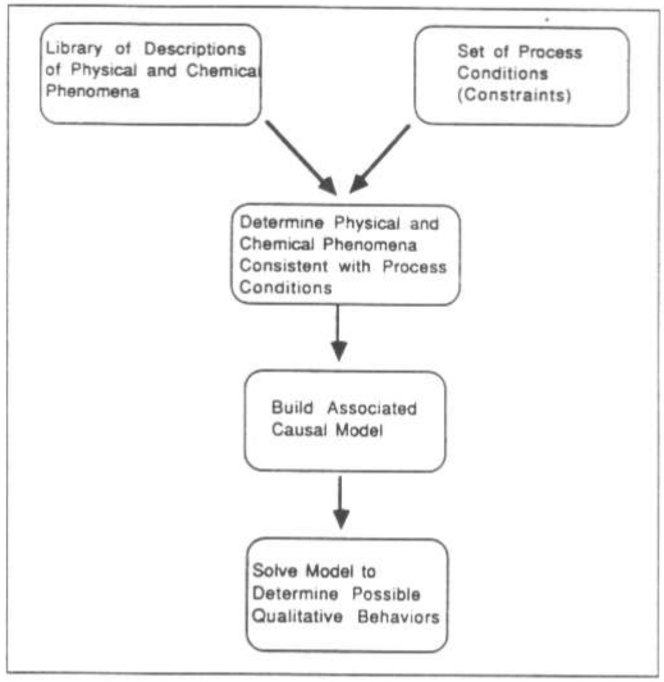

Figure 2b. Model building and solution using qualitative process theory.

For example, an increase in the time taken between entering the vaporizer and achieving boiling point would be described as $RC\text{-}DUR(T_0, T_1) = +$. Finally, let us define a transition variable, $TV(q, T_i)$, as a variable whose change of state is associated with the distinguished time point T_i. In the vaporizer example, there are two transition variables associated with the distinguished time point T_1: TV(temperature, T_1) and TV(boiling point, T_1).

Single-State Behavior

Mapping from changes in process conditions to changes in model

Our system is based on Forbus' qualitative process engine (QPE) (1988), which is an implementation of his qualitative process theory (QPT) (1984). This allows the definition of a set of fundamental physical and chemical phenomena (Figure 2a), which the system can use to build causal models from a physical description of the substances present and process conditions prevalent (Figure 2b). This enables the comparative analysis system to automatically change the constraints of the causal model to account for changes in process conditions.

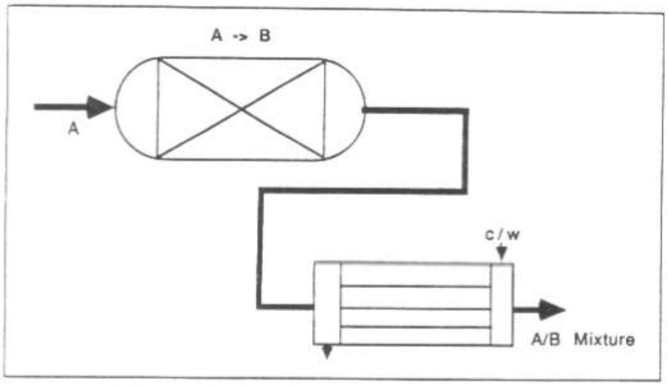

Figure 3. Product cooler scenario.

the changes in their starting values and derivatives. An example rule is:

If $QDIR(q, T_i, T_{i+1}) = +$ and if $RC\text{-}QDIR(q, T_i, T_{i+1}) = +$ and if not $RC\text{-}QS(q, T_i) = -$ and if not $RC-DUR(T_i, T_{i+1}) = -$ and if not $TV(q, T_{i+1})$ **then** $RC\text{-}QS(q, T_{i+1}) = +$

A complete set of rules, covering how all possible combinations of relative changes to starting values and derivatives affect the interval duration and end values, can be found in Appendix B, which also introduces the notation actually used in our code.

Case study 1: entrainment of catalyst into heat exchanger

Consider the case of catalyst being entrained into a product cooler shown in Figure 3. The behavior of the heat exchanger

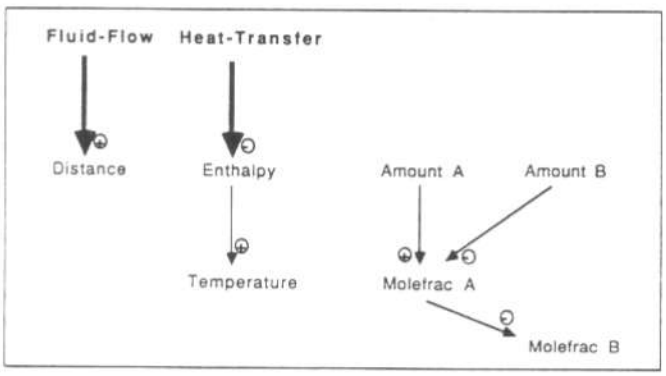

Figure 4a. Original model (no catalyst).

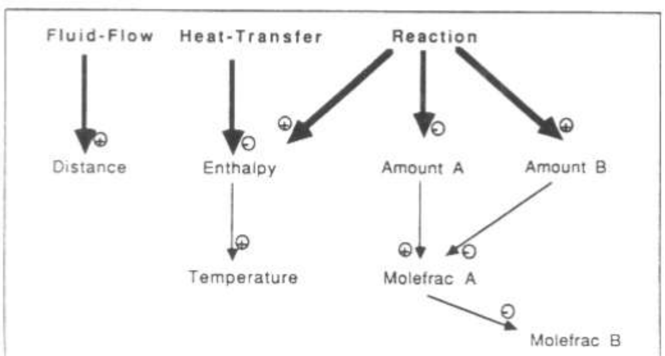

Figure 4b. New model (entrained catalyst).

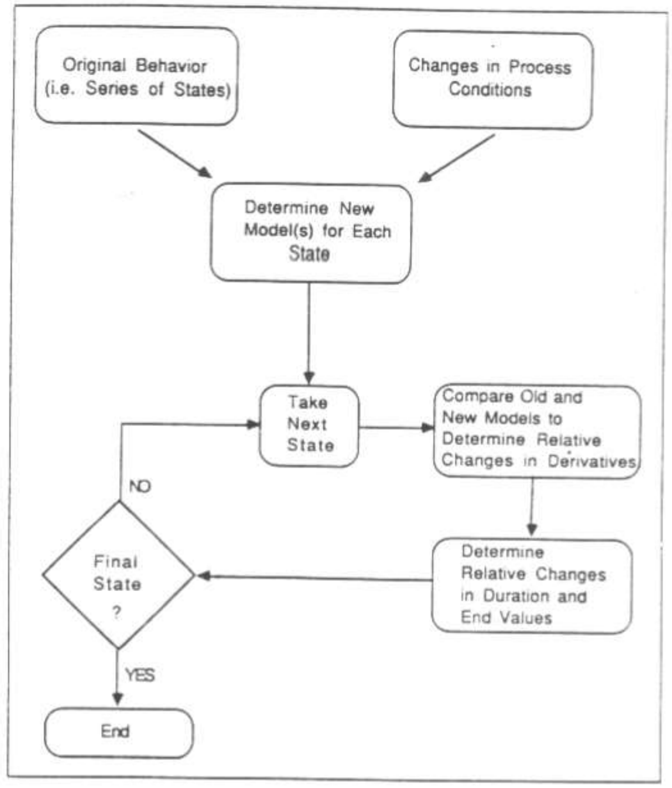

Figure 5. Comparative analysis assuming topological equivalence.

consists of a single-state description specified by the following conditions:

- Substance A contained in the tube side
- Substance B contained in the tube side
- A and B are miscible
- Temperature of the tube side < boiling point of A
- Temperature of the tube side < boiling point of B
- Temperature of the shell side < temperature of the tube side
- Pressure input > pressure output
- Distance < exit distance

These conditions imply the existence of three phenomena:

- The tube side contains a *two-component liquid.*
- There is *heat transfer* from the tube side to the shell side.
- There is *fluid flow* from the input to the output.

The associated model, describing the behavior of an elemental volume of fluid as it passes through the heat exchanger, is shown in Figure 4a. The solution of this model determines the signs of the parameter derivatives, as the elemental volume passes through the exchanger. The results are:

Tube-Side Parameter	$QDIR(q, T_0, T_1)$
Distance	+
Enthalpy	−
Temperature	−
Amount A	0
Amount B	0
Molefrac A	0
Molefrac B	0

The behavior terminates when the distance of the elemental volume along the exchanger increases to the exit distance, i.e., the alternative states are generated by removing the quantity conditions associated with the variables of interest and rerunning the model builder/solver. The resulting solutions will contain the original behavior together with all alternative behaviors.

The comparative analysis comprises the following stages:

1. Determine parameters to consider for transition (specified externally).

2. Remove quantity constraints associated with these parameters from the process condition specifications.

3. Perform limited envisionment to identify possible transitions and the new behaviors associated with these.

4. Filter out transitions not consistent with relative changes.

5. Match up intervals between new and original behaviors.

6. Compare behavior between matched intervals as described earlier.

Note that in many cases the new behavior may have a different number of intervals than the original one. To match up intervals in these circumstances it is necessary to split up a single interval into a number of "pseudo intervals" to give an equal number of intervals in each sequence. We use the heuristic that the interval to be split is always the last interval of the behavior with the least number of transitions. The relative change in duration associated with pseudo intervals is determined as if it had the same transition as the state to which it is compared.

Sometimes it is better to directly compare qualitative values of the final states rather than propagating relative changes from one state to the next. For example, consider a heater with an increased heat transfer coefficient causing the heated liquid to vaporize. Splitting and comparing the behaviors result in

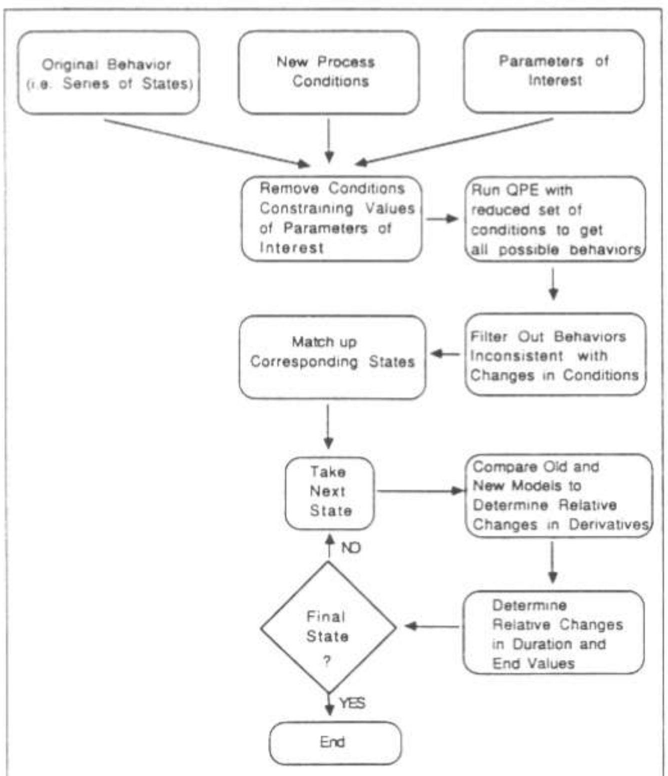

Figure 6. Comparative analysis assuming transition to new states.

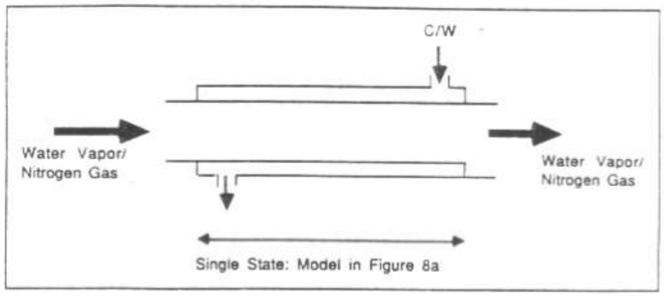

Figure 7a. Gas cooler.

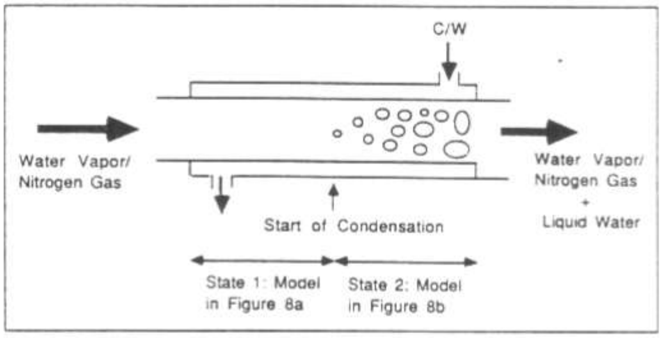

Figure 7b. Gas cooler after increase in tube-side pressure.

the new behavior having a higher temperature at the end of the first state; however, since it remains constant in the second state while the original behavior has its temperature increasing, it is not possible to determine which is ultimately higher! Obviously, by directly comparing qualitative states for temperature, one can determine that the new behavior has the higher exit temperature by virtue of it being at its boiling point. However, one must be careful when directly comparing final qualitative values, because these can change too. For example, if the pressure of the liquid is dropped so that it causes vaporization, the exit temperature of the new behavior may be lower than the original even though it is at its boiling point while the original is below its boiling point. The general rule followed in our system is to use matching of intervals and propagation of relative changes first and to try to resolve any resultant ambiguities using direct comparison of qualitative values providing the landmark value has not changed. A flowchart of the algorithm is shown in Figure 6.

Case study 2

Consider the heat exchanger shown in Figure 7a that cools a nitrogen/water gas mixture. The behavior is described by a single qualitative state characterized by the following process conditions:

- The tube side contains nitrogen.
- The tube side contains water.
- Temperature of the tube side > dew point of water.
- Temperature of the tube side > temperature of the shell side.
- Pressure inlet > pressure outlet.
- Distance < exit distance.

These conditions activate the following phenomena:

- The tube side contains a *two-component gas*.

the models for the two final states indicates that the new model has two new constraints associated with condensation and does not have the constraint relating temperature to enthalpy. The effects of these model changes are:

Tube-Side Parameter	$RC\text{-}QDIR(q, T_1, T_2)$
Enthalpy	0
Temperature	+
Distance	0
Amount of nitrogen in gas	0
Amount of water in gas	−
Molefrac of nitrogen in gas	+
Molefrac of water in gas	−

Since there is no relative change in the starting values of the final states, the relative changes of the end values (i.e., the exit values) are the same as in the above table for derivatives.

Thus, the comparative analysis has determined that a possible effect of increasing the operating pressure would be to induce condensation in the heat exchanger. The result of this is to produce a two-phase exit stream and to increase the exit temperature and increase the concentration of nitrogen in the exit gas phase.

Discussion

The comparative analysis system presented, which qualitatively predicts how changes in operating conditions affect the behavior of process units, has the unique ability of predicting the effect of changes in conditions that modify the underlying physics and chemistry of the situation and hence the appropriate qualitative model. This is achieved by combining the model creation and solution capabilities of Forbus' qualitative process engine with a model-model comparison system and modified rules from Weld's differential qualitative analysis technique.

In addition to its ability to analyze situations where the model changes, our comparative analysis system differs in several aspects from that of Weld. Weld's system produces answers to problems which have only one solution. When it is asked to determine the effect of multiple, competing changes, it returns without producing an answer. In contrast, our system produces all possible solutions together with the conditions under which each is appropriate. In addition, our system can deal with situations where the landmark values (the values at which parameters transition) change, whereas Weld assumes constant landmark values. Weld's system has the advantage of being able to reparameterize and analyze behavior from different perspectives. However, we developed our comparative analysis system for use in analyzing chemical plants where behavior is almost always viewed from the perspective of time (in batch processing units) or distance (in the case of continuous processing units). As such, our system implicitly considers behaviors only in terms of these perspectives.

Our system suffers from the same limitations associated with any qualitative representation in that it tends to produce multiple solutions for even very simple problems. This gets worse as the size of the chemical plant being reasoned about increases. This ambiguity arises from the weakness of qualitative representations and manifests itself in two ways: 1) inability to order transitions; and 2) inability to resolve multiple competing tendencies.

The first problem is circumvented by allowing the system to focus only on transitions associated with prespecified parameters. Unfortunately, the system still suffers from the second problem, which in general can only be solved with additional numerical information. The number of ambiguous solutions may possibly be reduced by adopting the techniques of D'Ambrosio (1987) or Kuipers and Berleant (1988).

The examples presented are for single pieces of equipment, but our comparative analysis technique is equally applicable to the analysis of a collection of units. The relative change at the end of one piece of equipment is simply taken as the input to the following piece of equipment. Due to the tendency of the technique to produce multiple solutions, analysis of groups of units (particularly systems with recycle loops) would not be practical with the procedure presented in this article. Such an analysis, however, may be possible when combined with techniques that reduce the complexity of models by focusing on specific areas of interest. Examples of focusing systems can be found in Falkenheiner and Forbus (1988) and Grantham (1990).

Recent work by Weld (Weld, 1990) shares our goal of analyzing model changes, but differs in several important aspects. First, Weld's approximation reformulation methodology deals specifically with the situation where the new model can be transformed into the old one (or *vice versa*) by approximating a single parameter to a limit. In contrast, our system can deal with multiple changes to modeling constraints as in the condenser example where the shift to a condensing regime changes the constraints affecting both temperature and the amount of liquid. Secondly, while Weld deals with the problem of selecting alternative possible models, it still requires *a priori* specification of the qualitative models themselves. Our system has the ability to automatically build and modify models, because it is built on top of Forbus' qualitative process engine.

Acknowledgment

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((**int-reverse ?a**) = **?b**)—The interval-duration value ?a is the reverse of the number ?b. Eg. ?a = increasing, ?b = − 1.

(**pos-ind-inf-by ?q1 ?q2 ?g**)—The relation (Qprop ?q1 ?q2) appears in the model of situation ?g.

(**neg-ind-inf-by ?z ?q ?g**)—The relation (Qprop- ?q1 ?q2) appears in the model of situation ?g.

(**lower-transition-var ?q**)—The quantity ?q is involved in the transition which ends the current interval and is the transition variable which had the lowest value prior to the transition.

(**upper-transition-var ?q**)—The quantity ?q is involved in the transition which ends the current interval and is the transition variable which had the highest value prior to the transition.

((**s (d ?q)**) = **?dir**)—The value of the quantity ?q is changing in the direction ?dir over the current interval. (Not to be confused with the change in derivative which is "delta-dir").

(**next-interval ?f ?g ?u ?i**)—The interval over which situations ?f and ?g are compared is immediately followed by the interval over which ?u and ?i are being compared.

Note that (lower-transition-var ?q), (upper-transition-var ?q) and (s (d ?q)) all refer to the new situation being compared. This distinction is required because the old and new situations do not necessarily have the same quantity behaviors or terminating transitions.

Rules

For the first interval duration only, propagate relative changes in start values to other start values. Limited to only one input change in starting value of first interval duration.

```
IF  Over (interval ?f ?g):
    (first-interval ?f ?g)
    ((start-value ?q) = ?v)
    ¬(equal ?v 0)
    (quantity ?z)
    (pos-ind-inf-by ?z ?q ?g)
    THEN
        ((start-value ?z) = ?v)
IF  Over (interval ?f ?g):
    (first-interval ?f ?g)
    ((start-value ?q) = ?v)
    ¬(equal ?v 0)
    (quantity ?z)
    (neg-ind-inf-by ?z ?q ?g)
    ((reverse ?v) = ?w)
    THEN
        ((start-value ?z) = ?w)
```

Determine change in interval duration lengths and end-values of transition parameters. These rules assume transition variables are not moving in the same direction.

```
IF  Over (interval ?f ?g):
    (lower-transition-var ?x)
    (upper-transition-var ?y)
    ((s (d ?x)) = ?z)
    ((s (d ?y)) = ?p)
    ¬(equal ?z ?p)
    ¬((delta-dir ?x) = 1)
    ¬((delta-dir ?y) = − 1)
    ¬((start-value ?x) = 1)
    ¬((start-value ?y) = − 1)
    (or((delta-dir ?x) = − 1)((start-value ?x) = − 1))
    THEN
        (interval-duration increase)
IF  Over (interval ?f ?g):
    (lower-transition-var ?x)
    (upper-transition-var ?y)
    ((s (d ?x)) = ?z)
    ((s (d ?y)) = ?p)
    ¬(equal ?z ?p)
    ¬((delta-dir ?x) = − 1)
    ¬((delta-dir ?y) = 1)
    ¬((start-value ?x) = − 1)
    ¬((start-value ?y) = 1)
    (or ((delta-dir ?x) = 1)((start-value ?x) = 1))
    THEN
        (interval-duration decrease)
IF  Over (interval ?f ?g):
    (lower-transition-var ?x)
    (upper-transition-var ?y)
    ((delta-dir ?x) = 0)
    ((delta-dir ?y) = 0)
    ((start-value ?x) = 0)
    ((start-value ?y) = 0)
    THEN
        (interval-duration stationary)
    AND
        ((end-value ?x) = 0)
    AND
        ((end-value ?y) = 0)
IF  Over (interval ?f ?g):
    (lower-transition-var ?x)
    (upper-transition-var ?y)
    ((s (d ?x)) = ?z)
    ((s (d ?y)) = ?p)
    ¬(equal ?z ?p)
    ¬((delta-dir ?x) = − 1)
    ¬((delta-dir ?y) = 1)
    ¬((start-value ?x) = − 1)
    ¬((start-value ?y) = 1)
    (or ((delta-dir ?y) = − 1)((start-value ?y) = − 1))
    THEN
        (interval-duration decrease)
IF  Over (interval ?f ?g):
    (lower-transition-var ?x)
    (upper-transition-var ?y)
    ((s (d ?x)) = ?z)
    ((s (d ?y)) = ?p)
    ¬(equal ?z ?p)
    ¬((delta-dir ?x) = 1)
    ¬((delta-dir ?y) = − 1)
    ¬((start-value ?x) = 1)
    ¬((start-value ?y) = − 1)
    (or ((delta-dir ?y) = 1)((start-value ?y) = 1))
    THEN
        (interval-duration increase)
```

Rule for when we get competing changes in transition variables/start-values giving 3 possibilities for internal change

```
IF  Over (interval ?f ?g):
    (upper-transition-var ?x)
    ((start-value ?x) = ?y)
    ((delta-dir ?x) = ?b)
```

((reverse ?z) = ?y)
((delta-dir ?x) = ?e)
¬(equal ?e ?y)
THEN
((end-value ?x) = ?z)

IF Over (interval ?f ?g):
(interval-duration stationary)
(quantity ?x)
((delta-dir ?x) = 0)
((start-value ?x) = 0)
THEN
((end-value ?x) = 0)

Rules for situations when get multiple possible outcomes

IF Over (interval ?f ?g):
(quantity ?x)
((delta-dir ?x) = ?a)
((start-value ?x) = ?b)
((reverse ?a) = ?b)
THEN EITHER
((end-value ?x) = 0)
OR
((end-value ?x) = 1)
OR
((end-value ?x) = −1)

IF Over (interval ?f ?g):
(quantity ?x)
(interval-duration ?y)
((start-value ?x) = ?b)
((int-reverse ?y) = ?b)
THEN EITHER
((end-value ?x) = 0)
OR
((end-value ?x) = 1)
OR
((end-value ?x) = −1)

IF Over (interval ?f ?g):
(quantity ?x)
(interval-duration ?y)
((delta-dir ?x) = ?b)
(int-reverse ?y) = ?b)
THEN EITHER
((end-value ?x) = 0)
OR
((end-value ?x) = 1)
OR
((end-value ?x) = −1)

Rule that states that end-values of previous interval are start-values of next.

IF Over (interval ?f ?g):
(next-interval ?f ?g ?u ?i)
((end-value ?x) = ?v)
THEN
((start-value ?x) = ?v) Over (interval ?u ?i)

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