Contributed Paper

Qualitative-model Simplification with an Application to Multistage Separation Processes

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Deep-model-based qualitative reasoning provides a systematic framework for describing qualitative physical phenomena. However, as physical systems become more and more complex, the computational load and complexity of qualitative simulation increase dramatically. Multistage separation processes are among the most important unit operations in chemical engineering. An industrial-scale multistage separation process is normally described by some tens or hundreds of quantitative equations. Qualitative reasoning for this type of process is difficult, if not impossible. Since multistage separation processes are highly structured (e.g. cascaded stages), the concept of model simplification (or model reduction), often seen in the practice of process control, is applied to qualitative modeling. The objective of this work is to simplify the qualitative process model according to the structural properties of the multistage separation processes. The simplified qualitative model can, on the one hand, reduce the computational load in qualitative simulation and, on the other hand, retain the qualitative description of the system. In this work, the simplest qualitative model, the signed directed graph (SDG), is used and the most common multistage separation process, using distillation columns, is studied. Qualitative simulation results show that qualitative-model simplification offers an attractive approach for reasoning about important, practical problems.

Keywords: Qualitative model, signed directed graph, model reduction, separation process.

1. INTRODUCTION

Recently, qualitative physics¹⁻³ has received a great deal of attention in the field of artificial intelligence. It provides a systematic approach for describing physical phenomena in a qualitative manner, e.g. increase, decrease or no change.

Similar to the quantitative process description, qualitative reasoning consists of two stages: modeling and simulation. At the modeling stage, qualitative relationships between process variables are established. The qualitative relationships may be of various forms: algebraic, linguistic, graphical representations, etc. In qualitative physics, typical modeling approaches include: ENVISION arithmetic or confluences,⁴ qualitative constraints or QSIM,⁵ qualitative process theory,⁶ and SR1.⁷ After the model has been constructed, the behavior can be derived from a simulation (e.g. find the

consistent behavior). In chemical engineering applications of qualitative physics can be found in trouble-shooting⁸ and fault diagnosis.^{9,10}

In the modeling stage, the quantitative differential and algebraic equations can be relaxed into qualitative ones. That is, the precise quantitative value becomes a qualitative one, e.g. increase(+), decrease(−) or no change(0). This step may cause ambiguity in the description of the behavior. However, the applicability of the model increases significantly, since much less knowledge (only qualitative information) is required. This is especially useful in engineering applications, since the qualitative process knowledge can be obtained over years of process operation.

Separation is one of the most important unit operations in chemical engineering. A typical separation process takes the form of a multistage operation. In other words, it is constructed by means of many repeated sub-units, so as to reach the desired separation. Typical multistage operations include: absorption, extraction, distillation, etc.¹¹ In the case of distilla-

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tion, an industrial-scale column consists of some tens or hundreds of serial sub-units.¹² The number of stages for a multistage separation process in a chemical plant ranges from some tens to hundreds. For a binary distillation column, the number of "quantitative" differential equations employed in describing this system are about twice the number of its tray. For example, for a 80-tray binary column, at least 160 differential equations are required. One can relax these equations to find the corresponding qualitative ones (e.g. a model with 160 qualitative differential equations). Obviously, it is impractical to solve the model to derive any physical behavior. However, it is well known (to chemical engineers) that cascade multistage separation processes are highly structured. Therefore, the structure of the process can be utilized to simplify the qualitative model. The purpose of this work is to provide a systematic approach to simplifying the qualitative model of the highly structured multistage separation process. The process being studied is the familiar distillation column, and the qualitative model of interest is the simplest qualitative model: a signed directed graph (SDG). Furthermore, the qualitative-model simplification procedure is also illustrated using algebraic expressions (the ENVISION arithmetic, to be specific).

This paper is organized as follows. Section 2 reviews the qualitative physics and an introduction to the SDG model is given, followed by the principles employed in model simplification. The algebraic counterpart (as opposed to the graphical SDG approach) of the qualitative-model simplification is also given. Distillation columns are introduced in Section 3, and the model simplification procedure is illustrated. The results of quantitative simulation, and qualitative simulations of the full and simplified qualitative models are given in Section 4, followed by the conclusions.

2. QUALITATIVE REASONING: A SIGNED DIRECTED GRAPH APPROACH

2.1. The use of SDG to represent physical phenomena

Signed Directed Graphs (SDG) have a long history of successful applications in the field of engineering.^{9,13-16} The SDG consists of three components: node, directed branch and sign.¹⁴ In SDG, a node corresponds to a process variable in the form of a deviation variable, and a branch represents the immediate influence between two nodes. Whether an influence is positive or negative is distinguished by the sign "+", "-", or "0" in SDG. These indicate whether the current value of the variable is "higher than, lower than, or equal to" its nominal value. One advantage of using SDG to represent a physical system is that one can "visualize" how the system behaves.

2.2. Qualitative modeling based on SDG

The SDG of a chemical process can be constructed from Ref. 14:

- (1) plant data and/or an operator's experience;
- (2) a mathematical model of the process.

The SDG constructed from the latter approach will generally yield a more complete description of the process if the model is reasonably complete. Typically, a mathematical model may include algebraic and ordinary differential equations. The SDG model can be derived from a linearized version of the process model in a straightforward manner. The linearized equation, with variables expressed in the form of deviation variables, can be expressed as:

$$\frac{dx_i}{dt} = \sum_{j=1}^n a_{ij} \cdot x_j \quad (1)$$

$$x_i = \sum_{j=1}^n b_{ij} \cdot x_j. \quad (2)$$

An SDG model can be constructed as follows: x_i is the terminal node. The sign of the branch is the same as that of a_{ij} or b_{ij} from the corresponding equation. In this work, the qualitative SDG model is constructed in accordance with its mathematical model.

2.3. Qualitative simulation based on SDG

The procedure of inference by experts is commonly a forward-reasoning process. In other words, a disturbance (change in the variable) is made to the nominal system, and the result can be derived according to the SDG. Initially, the process is at the steady-state, and the state of all variables is "0". As a disturbance occurs, the effect propagates through the branches. This results in changes in the subsequent nodes, until the ultimate steady-state is reached. In this paper, the SDG is used to describe the steady-state or quasi-steady-state behavior of a system.

The operation for building an SDG model is straightforward. The state of the terminal node is determined by multiplying the state of the initial node by the sign of the branch. For example, in the following SDG:

$$A \xrightarrow{\text{sgn}(A-B)} B$$

the state of node B is

$$[B] = \text{sgn}(A-B) \cdot [A], \quad (3)$$

where $\text{sgn}(A-B)$ represents the sign of the branch, $[A]$ is the state of the initial node A , and $[B]$ is the state of the terminal node B .

Once a measurement pattern (qualitative states of A and B) is available, the branch

$$A \xrightarrow{\text{sgn}(A-B)} B,$$

is said to be "consistent" if the states of A and B agree with equation (3). The pattern means a set of qualitative states for a corresponding SDG. For the

Table 1. Truth tables

$A \xrightarrow{+} B$			
B			
A	+	0	-
+	T	F	F
0	F	T	F
-	F	F	T

$A \xrightarrow{-} B$			
B			
A	+	0	-
+	F	F	T
0	F	T	F
-	T	F	F

SDG-model-based qualitative simulation, if all the branches in an SDG are consistent with a given pattern, then the pattern is a “solution” to the SDG model. Since there are only two basic branch types, $A \xrightarrow{+} B$ and $A \xrightarrow{-} B$, the truth tables (Table 1) can be defined to discriminate the inconsistent branches for a given measurement pattern. At the programming level, logical operators p and m are defined to describe these two types of branches:

$$(pAB) \Leftrightarrow A \xrightarrow{+} B \quad (4)$$

$$(mAB) \Leftrightarrow A \xrightarrow{-} B. \quad (5)$$

Thus the result of a logical operation takes the value of “true” or “false”, determined from the truth tables, given the measurement pattern and the corresponding SDG Model.

In the implementation phase, many “subgraphs” can be derived from the SDG model for many possible perturbations, and logical rules, for qualitative simulation, are developed for all its subgraphs. Several principles can be applied as the guide-lines for rule writing.^{15,16} The first case is that several pathways converge to a single node. If the node n_i is influenced by the nodes $K_1, K_2, \dots$, and K_j , the premise of node n_i can be written as a clause.⁵

$$[(*K_1 n_i) .\text{or.} (*K_2 n_i) .\text{or.} , \dots , .\text{or.} (*K_j n_i)] \quad (6)$$

where $K_j (j=1, 2, \dots, J)$ are the immediate input nodes to n_i , and $*$ represents the logical functions p or m .

For each node, the premise can be written and the overall premise of an SDG is simply the combination of the clauses of all nodes via the .and. operator:

$$(\text{clause of } n_1) .\text{and.} (\text{clause of } n_2) .\text{and.} , \dots , .\text{and.} (\text{clause of } n_i) \quad (7)$$

where $n_i (i=1, 2, \dots, I)$ is the i th node in the SDG. The statements in (6) and (7) show the “general” way to implement SDG rules.

2.4. Model simplification—graphical approach

Two principles are utilized for the simplification of an SDG. One is the principle of “removal of intermediate nodes” and the other is the “simplification of the positive feedback loop”.

2.4.1. Removal of intermediate nodes

Removed nodes, in most cases, correspond to variables that are unimportant, or intermediate variables in a system. One important criterion is that the qualitative description of the variables of interest should remain the same after the simplification procedure. “Removal of intermediate nodes” is fundamentally similar to the principle “removal of unmeasured nodes”^{9, 15, 16} which is frequently employed in diagnostic problems. The principle is simple. A new branch is formed after the removal of an intermediate node. The sign of this new branch is determined by multiplying the signs of the original branches. For example, for an SDG,

$$A \xrightarrow{\text{sgn}(A-B)} B \xrightarrow{\text{sgn}(B-C)} C,$$

if the intermediate node, B , is removed, then the sign of the new branch,

$$A \xrightarrow{\text{sgn}(A-C)} C,$$

becomes:

$$\text{sgn}(A-C) = \text{sgn}(A-B) \cdot \text{sgn}(B-C). \quad (8)$$

This can be applied to a more complex situation. Figure 1(A) shows the original SDG of a *single*-tray distillation column which describes the causal effects between the feed composition x_f , top product composition x_D and bottoms product composition x_B as well as bottoms vapor composition y_B and the compositions in tray 1, i.e. x_1 and y_1 . The “removal of intermediate nodes” principle can be applied as follows. First, since the vapor phase compositions y_1 and y_B are of no interest, the corresponding nodes, Y_1 and Y_B , can be treated as intermediate nodes. Y_1 and Y_B can be removed in a straightforward manner [Fig. 1(B)]:

$$X_1 \xrightarrow{+} Y_1 \xrightarrow{+} X_D \Leftrightarrow X_1 \xrightarrow{+} X_D$$

$$X_B \xrightarrow{+} Y_B \xrightarrow{+} X_1 \Leftrightarrow X_B \xrightarrow{+} X_1.$$

Since the qualitative values of X_D and X_B are of interest, a further step can be taken, to remove X_1 . Applying the same principle, a simplified SDG model is derived [Fig. 1(C)]. It is important to note that the simplified SDG has the same behavioral description for the variables X_f, X_D and X_B as the full SDG.

2.4.2. Simplification of a positive feedback loop

In an SDG, “feedback loop” means that a perturbation in one node will propagate back to itself via

some other nodes. To avoid spurious solutions, it is suggested by Kramer and Palowitch¹⁵ that extra clauses are needed. Since the SDG of any multistage separation process has included many positive feedback loops, the method is modified to avoid spurious solutions without adding extra clauses.

A. Single positive feedback loop. Figure 1(C) shows a positive feedback loop between B and C. Following the general procedure, the rule can be written as:

$$\begin{aligned} \text{IF } [X_F = +] \text{ .and. } [(pX_F X_D) \text{ .or. } (pX_B X_D)] \\ \text{ .and. } [(pX_F X_B) \text{ .or. } (pX_D X_B)] \\ \text{ THEN it is a possible solution pattern} \\ \text{ for a positive change in } X_F, \end{aligned} \quad (9)$$

The exact solution for this example should be $X_F = X_D = X_B = +$. But the general rule also produces the spurious solution $X_D = X_B = -$. This means the positive feedback loop is isolated from the entire graph.

Since all the nodes in a positive feedback loop take the same qualitative value (which is the same as the effect of external forcing), the spurious solutions can be

eliminated by removing the positive feedback nodes in Fig. 1(C). Therefore, the qualitatively correct description for the positive feedback loop can be described in a much simpler form:

$$\begin{aligned} \text{IF} \\ [X_F = +] \text{ .and. } [(pX_F X_D) \text{ .and. } (pX_F X_B)] \\ \text{ THEN} \\ \text{it is a possible solution pattern} \\ \text{for a positive change in } X_F \end{aligned} \quad (10)$$

B. Cascaded positive feedback loops. Typical multistage separation processes are more complex than that shown in Fig. 1. They generally consist of many positive feedback loops in cascade, as shown in Fig. 2(A). Figure 2(A) shows an SDG with three positive feedback loops, e.g. B & C, C & D and D & E. These loops share some common nodes (C and D). The term "cascaded positive feedback loops" is used to describe these cascaded loops. The principle of "removal of intermediate nodes" can be applied to derive direct effects from node A to node B, C, D and E. The procedure is similar to the one described earlier. This

Fig. 1. Simplification of SDG for a given external disturbance X_F . (A) original SDG; (B) removal of Y_1 , Y_B ; (C) removal of X_1 .

Fig. 2. (A) SDG for cascaded positive feedback loops; (B) simplified SDG as an equivalent description of (A).

greatly simplifies the rule in describing the phenomena [Fig. 2(B)]:

IF

$$[A = +] \text{ .and. } [mAB] \text{ .and. } [mAC] \\ \text{ .and. } [mAD] \text{ .and. } [mAE]$$

THEN

it is a possible solution pattern for

a positive change in A (11)

2.5. Model simplification—algebraic approach

Algebraic forms of qualitative models have received a great deal of attention recently, e.g. the ENVISION arithmetic of de Kleer and Brown,⁴ and QSIM of Kuipers.⁵ The algebraic counterpart of qualitative-model simplification is illustrated. de Kleer and Brown's ENVISION is used to show the model simplification procedure. An extension to some other method is straightforward. Two corresponding algebraic manipulations are needed. One is "direct substitution", and the other is "further simplification".

2.5.1. Direct substitution

Consider the single-tray distillation column example in Fig. 1(A). The confluences describing this system are:

$$[X_D] = [Y_1] \quad (12)$$

$$[X_1] = [X_D] + [Y_B] + [X_f] \quad (13)$$

$$[Y_1] = [X_1] \quad (14)$$

$$[X_B] = [X_1] \quad (15)$$

$$[Y_B] = [X_B]. \quad (16)$$

Substituting (14) and (16) into (12) and (13), respectively,

$$[X_D] = [X_1] \quad (17)$$

$$[X_1] = [X_D] + [X_B] + [X_f] \quad (18)$$

$$[X_B] = [X_1]. \quad (19)$$

This is exactly the simplified system shown in Fig. 1(B). A further step can be taken by eliminating the node X_1 using direct substitution. Substituting (18) into (17) and (19),

$$[X_D] = [X_D] + [X_B] + [X_f] \quad (20)$$

$$[X_B] = [X_D] + [X_B] + [X_f]. \quad (21)$$

The confluences [(20) and (21)] describe a system very similar to the simplified SDG in Fig. 1(C), except that self-loops exist in the nodes X_D and X_B (loops starting and ending at the same node). Equations (20) and (21) can be simplified by eliminating $[X_D]$ and $[X_B]$ in (20) and (21), respectively. Appendix B gives the justification for this simplification step. This step is denoted as "self-elimination" in the discussion which follows. Therefore, the confluences become:

$$[X_D] = [X_B] + [X_f] \quad (22)$$

$$[X_B] = [X_D] + [X_f], \quad (23)$$

Equations (22) and (23) are equivalent to the system described by Fig. 1(C). In terms of SDG, the difference between (20) & (21) and (22) & (23) is the removal of the self-loop. It is well-known that a self-loop can be removed without generating spurious solution.

2.5.2. Further simplification

In the SDG counterpart, the next step is to break the positive feedback loop into tree structures. In the form of ENVISION arithmetic, this can be accomplished using the same principles: direct substitution and self-elimination. Substituting (23) into (22),

$$[X_D] = [X_D] + [X_f] + [X_f]. \quad (24)$$

It is obvious that (24) can be reduced to:

$$[X_D] = [X_D] + [X_f]. \quad (25)$$

Applying the principle of self-elimination, equation (25) becomes:

$$[X_D] = [X_f]. \quad (26)$$

Similarly, by substituting (22) into (23),

$$[X_B] = [X_f]. \quad (27)$$

Equations (26) and (27) are exactly the results of "simplification of the feedback loop" as shown in (10).

Clearly, this section illustrates the algebraic counterpart of qualitative-model simplification. The two basic operations employed are direct substitution and self-elimination (Appendix B). Technically, the operations employed in the qualitative-model simplification procedure are closely related to qualitative algebras.^{7, 17, 18} Obviously, the applicability of the simplification procedure is not limited to multistage separation processes.

3. QUALITATIVE-MODEL SIMPLIFICATION FOR DISTILLATION COLUMNS

3.1. Quantitative model

The distillation column is one of the most common separation units in chemical process industries. The function of a distillation column is to separate mixtures of light and heavy components. Most of the light component comes out from the top of the column (D) and the heavy component goes out from the bottoms (B) as shown in Fig. 3. The reflux flow rate (L) and the vapor boilup (V) are manipulated to maintain the desired product specifications. This is known as the L - V structure.^{11, 18, 20}

Figure 3 shows an nt -tray distillation column. In Fig. 3, F , D and B denote the feed, distillate and bottoms flow rates and x_f , x_D and x_B are the mole fractions of the light component in the feed, distillate and bottoms. x_i and y_i are the liquid and vapor phase compositions in the i th tray and y_B is the vapor phase composition in the bottoms. M_i , M_D and M_B are holdups in the i th tray, reflux drum and bottoms. It can be divided into five sections (Fig. 3):

- (1) reboiler;
- (2) stripping section (from tray 1 to tray $nf-1$);
- (3) feed tray (tray nf);
- (4) rectifying section (from tray $nf+1$ to tray nt);
- (5) condenser.

Before developing the quantitative model (differential and algebraic equations), the following basic assumptions are made:

- (1) binary mixture;
- (2) saturated liquid feed;
- (3) total condenser and partial reboiler;
- (4) equal molar overflow;
- (5) perfect level control in both the reflux drum and bottom.

The differential and algebraic equations describing the vapor liquid equilibrium and material balances are derived. For an nt -tray column, this accounts for $(nt+2)$ differential equations and $(nt+3)$ algebraic equations. Similar models can be found elsewhere.^{19, 20}

3.2. Qualitative model

In this work, the qualitative model is derived from a quantitative model. It should be noticed that not all forms of quantitative model lead to an appropriate (simple) qualitative model, since different expressions in the quantitative model may result in different qualitative models for the same process. Therefore, algebraic manipulations are necessary to arrive at the simplest form of a qualitative model.

A linearized distillation model can be derived (Appendix A from the full distillation model).²⁰ In Appendix A, the characters with an upper bar, " $\bar{}$ ", are steady-state values, and the rest of the variables are perturbation variables. For a distillation column with an L - V structure, four variables, F , x_f , L and V are considered as independent variables. The first two, F and x_f , are known as external disturbances, and the latter two are the manipulated variables (which can be changed to maintain product specifications). Product

Fig. 3. A typical nt -tray distillation column with single feed and two product streams.

Fig. 4. Overall SDG model of an nt -tray distillation column.

compositions (x_D and x_B), bottoms vapor composition (y_B), compositions on each tray (x_s and y_s), and top and bottoms flow rates (D and B) are all influenced as these four variables change. The equations in Appendix A provide the basis for deriving the SDG model.

Several characteristics of distillation columns are useful in deriving the qualitative model:

- (1) on each tray, the mole fraction of the light component in the vapor phase is higher than that of the liquid phase, i.e. $\bar{y}_B > \bar{x}_B$, and $\bar{y}_i > \bar{x}_i$.
- (2) at steady-state, the mole fraction of the light component on the upper tray is higher than that of the lower one, i.e. $\bar{x}_D > \bar{x}_{nt} > \dots > \bar{x}_{nf} > \dots > \bar{x}_1 > \bar{x}_B$ and $\bar{y}_{nt} > \dots > \bar{y}_{nf} > \dots > \bar{y}_1 > \bar{y}_B$.
- (3) all variables have positive numerical values, and $(L + F) > V$.

Using this common-sense knowledge, the SDG model can readily be derived from Appendix A. The SDG model is shown in Fig. 4. Note that, in Fig. 4, branches with dotted lines, " $\cdots \rightarrow$ ", are used to denote the negative branches, " $\bar{\rightarrow}$ ". The branches with solid lines, " $\rightarrow$ ", represent the positive branches,

" $\rightarrow$ ". Furthermore, no branch goes into the four independent variables F and L (Fig. 4). This means that those four variables affect the rest of the V , X_f , variables, but the opposite is not true. One important observation is that there are $(nt + 1)$ cascaded positive feedback loops (Fig. 4). This model is a highly structured SDG model. Actually, this phenomenon is quite common for multistage separation processes, since repeated units (performing the same function) are used to achieve the desired product purity.

Consider a 10-tray distillation column with the feed at tray 5 ($nf=5$) as an example. The "overall SDG model" is shown in Fig. 5. With the $L-V$ structure, the four independent variables are, again, V , X_f , F and L . Sub-models describing the effect of each independent variable can also be derived from Fig. 5. For example, to investigate the qualitative phenomena when F changes, the subgraph can be constructed by eliminating the nodes and branches which cannot be reached from F (i.e. eliminating the nodes D , V , X_f , L and associated branches in Fig. 5).

3.3. Model simplification

From the structure of the SDG model (Fig. 5), it is clear that the SDG can be simplified significantly if

one's interest is the top and bottoms compositions (X_D and X_B). The principle of "removal of intermediate nodes" is useful in the simplification steps.

- (1) removing all intermediate Y_i nodes except Y_5 (the vapor phase composition in the feed tray);
- (2) removing all intermediate X_i nodes except X_5 (liquid phase composition in the feed tray) (Fig. 6).

Following these two steps, a minimal model (Fig. 6) is derived for a behavioral description. Actually, the model simplification can be applied to columns with different tray numbers (e.g. $nt=1,2,3,\dots$). However, the resultant minimal models are exactly the same, except that the subscript 5 in Fig. 6 is replaced by the corresponding feed tray (i.e. nf) in Fig. 6. For example, a 190-tray column separating propane and propylene (a C_3 splitter of Exxon chemicals) with the feed on tray 61²¹ can be described qualitatively using Fig. 6 (replacing the subscripts 5 with 61 in Fig. 6). This implies that, qualitatively, the behavior of a 1-tray distillation column is no different from a 190-tray column. However,

Fig. 5. Overall SDG model of a 10-tray distillation column.

Fig. 6. Simplified SDG model obtained by eliminating all X_i 's and Y_i 's except X_5 and Y_5 .

quantitatively, a 190-tray column is quite different from a single-tray column. The findings from qualitative-model simplification coincide with the physical intuition of most chemical engineers.

Furthermore, a nt -tray column can be simplified into the equivalent form of Fig. 6 (with X_5 and Y_5 replaced with X_{nf} and Y_{nf}) using the procedure illustrated in

Table 2. Qualitative behavior from quantitative simulation for a 10-tray distillation column with a positive change in L .

*** P : A Positive Change (10%)

L	P	+	+	+	+	+	+	+	+	+
V	0	0	0	0	0	0	0	0	0	0
F	0	0	0	0	0	0	0	0	0	0
Xf	0	0	0	0	0	0	0	0	0	0
D	0	-	-	-	-	-	-	-	-	-
B	0	+	+	+	+	+	+	+	+	+

Time 0 1 2 3 4 5 6 7 8 9 (min)

XD	0	+	+	+	+	+	+	+	+	+
X1	0	+	+	+	+	+	+	+	+	+
X2	0	+	+	+	+	+	+	+	+	+
X3	0	+	+	+	+	+	+	+	+	+
X4	0	+	+	+	+	+	+	+	+	+
X5	0	+	+	+	+	+	+	+	+	+
X6	0	+	+	+	+	+	+	+	+	+
X7	0	+	+	+	+	+	+	+	+	+
X8	0	+	+	+	+	+	+	+	+	+
X9	0	+	+	+	+	+	+	+	+	+
X10	0	+	+	+	+	+	+	+	+	+
XB	0	+	+	+	+	+	+	+	+	+

Time 0 1 2 3 4 5 6 7 8 9 (min)

Y1	0	+	+	+	+	+	+	+	+	+
Y2	0	+	+	+	+	+	+	+	+	+
Y3	0	+	+	+	+	+	+	+	+	+
Y4	0	+	+	+	+	+	+	+	+	+
Y5	0	+	+	+	+	+	+	+	+	+
Y6	0	+	+	+	+	+	+	+	+	+
Y7	0	+	+	+	+	+	+	+	+	+
Y8	0	+	+	+	+	+	+	+	+	+
Y9	0	+	+	+	+	+	+	+	+	+
Y10	0	+	+	+	+	+	+	+	+	+
YB	0	+	+	+	+	+	+	+	+	+

Time 0 1 2 3 4 5 6 7 8 9 (min)

Table 3. Rules for the full and the simplified models for the 10-tray distillation column

* Full SDG model		

* SDG Rule :		

* IF [L = +] .and. { mLD } .and. { pLB }		
* .and. { pLXB } .and. { pXBYB }		
* .and. { pLX1 } .and. { pX1Y1 }		
* .and. { pLX2 } .and. { pX2Y2 }		
* .and. { pLX3 } .and. { pX3Y3 }		
* .and. { pLX4 } .and. { pX4Y4 }		
* .and. { pLX5 } .and. { pX5Y5 }		
* .and. { pLX6 } .and. { pX6Y6 }		
* .and. { pLX7 } .and. { pX7Y7 }		
* .and. { pLX8 } .and. { pX8Y8 }		
* .and. { pLX9 } .and. { pX9Y9 }		
* .and. { pLX10 } .and. { pX10Y10 }		
* .and. { pY10XD }		

* THEN it is a possible solution pattern for		
* a positive change in L		

=====		

* Simplified SDG model		

* SDG Rule :		

* IF [L = +] .and. { mLD } .and. { pLB }		
* .and. { pLXB } .and. { pXBYB }		
* .and. { pLX5 } .and. { pX5Y5 }		
* .and. { pLXD }		

* THEN it is a possible solution pattern for		
* a positive change in L		

Section 2.5. if the algebraic expression is preferred. Section 2.5 gives the details of the algebraic manipulations.

4. PROCESS SIMULATION AND QUALITATIVE SIMULATION

The results derived in Section 3 are illustrated via simulations. Comparisons are made between quantitative process simulation, qualitative simulation of the full model and qualitative simulation of the simplified model. The basis for comparison is the qualitative behavior of a distillation column. A 10-tray distillation column, with feed at the 5th tray, is used to illustrate these comparisons.

4.1. Process simulation

A nonlinear tray-by-tray dynamic model is developed for the 10-tray column. The column is simulated for a positive change (10%) in the reflux flow rate L . The results of the quantitative simulation are transformed into qualitative states, “+”, “-” or “0”. Table 2 describes the qualitative behavior (from quantitative simulation) for all the process variables for a step change in L .

4.2. Qualitative simulation

The qualitative model for the 10-tray column is shown in Fig. 5 (the full model) as well as Fig. 6 (the

simplified model). Logic rules can also be written for the full model and the simplified model (Table 3). It is obvious that a much simpler set of rules is used for the simplified model. Furthermore, the difference becomes larger as the number of trays increases. The results of qualitative simulations (consistent patterns) for the full model and the simplified model are exactly the same for the qualitative states of interest. The results presented here show that, as far as qualitative behavior is concerned, the simplified qualitative model is sufficient.

5. CONCLUSION

The concept of model simplification or model reduction is a common practice in the field of process control when dealing with quantitative process models. In the work, an approach for qualitative-model simplification is proposed. The idea is carried out using the simplest qualitative model: the Signed Directed Graph (SDG). Model-simplification is based on the principles: “removal of intermediate nodes” and “simplification of positive feedback loop”. It is shown to be useful in finding the qualitative behavior of the multistage separation processes which are the most important units in chemical process industries. For industrial-scale distillation columns, qualitative reasoning is difficult, if not impossible. Using the concept of qualitative-model sim-

plication, reasoning about the behavior of a industrial-scale column is as simple as that of the simplest column, i.e. a single-tray column. Simulation results show that the simplified qualitative model possesses the same quality (in behavior description) as the full model at a level of much less computing effort. The results presented here are generally applicable to a wide class of multistage separation processes. Furthermore, the concept of qualitative-model simplification is also illustrated using the more familiar qualitative model (e.g. qualitative models in algebraic form, ENVISION arithmetic). Basic operations for the simplification procedure are also given.

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APPENDIX A

Linearized Model for a *nt*-Tray Column

(i) Partial reboiler

$$B = L + F - V$$

$$\dot{X}_B = \{(\bar{x}_1 - \bar{x}_B)(L + F) + (\bar{x}_B - \bar{y}_B)V + (\bar{L} + \bar{F})X_1 - (\bar{L} + \bar{F} - \bar{V} + \bar{K}_B \bar{V})X_B\} / \bar{M}_B$$

$$Y_B = \bar{K}_B X_B$$

(ii) Stripping section

$$\dot{X}_1 = \{(\bar{x}_2 - \bar{x}_1)(L + F) + (\bar{y}_B - \bar{y}_1)V + (\bar{L} + \bar{F})X_2 + \bar{V}Y_B - (\bar{L} + \bar{F} + \bar{K}_B \bar{V})X_1\} / \bar{M}_1$$

$$Y_1 = \bar{K}_1 X_1$$

⋮

$$\dot{X}_{nf-1} = \{(\bar{x}_{nf} - \bar{x}_{nf-1})(L + F) + (\bar{y}_{nf-2} - \bar{y}_{nf-1})V + (\bar{L} + \bar{F})X_{nf} + \bar{V}Y_{nf-2} - (\bar{L} + \bar{F} + \bar{K}_{nf-1} \bar{V})X_{nf-1}\} / \bar{M}_{nf-1}$$

$$Y_{nf-1} = \bar{K}_{nf-1} X_{nf-1}$$

(iii) Feed location

$$\dot{X}_{nf} = \{(\bar{x}_{nf+1} + \bar{x}_{nf})L + (\bar{x}_f - \bar{x}_{nf})F + (\bar{y}_{nf})V + \bar{F}X_f + \bar{L}X_{nf+1} + \bar{V}Y_{nf-1} - (\bar{L} + \bar{F} + \bar{K}_{nf} \bar{V})X_{nf}\} / \bar{M}_{nf}$$

$$Y_{nf} = \bar{K}_{nf} X_{nf}$$

(iv) Rectifying location

$$\dot{X}_{nf+1} = \{(\bar{x}_{nf+2} - \bar{x}_{nf+1})L + (\bar{y}_{nf} - \bar{y}_{nf+1})V + \bar{L}X_{nf+2} + \bar{V}Y_{nf} - (\bar{L} + \bar{K}_{nf+1} \bar{V})X_{nf+1}\} / \bar{M}_{nf+1}$$

$$Y_{nf+1} = \bar{K}_{nf+1} X_{nf+1}$$

⋮

$$\dot{X}_{nt} = \{(\bar{x}_D - \bar{x}_{nt})L + (\bar{y}_{nt-1} - \bar{y}_{nt})V + \bar{L}X_D + \bar{V}Y_{nt-1} - (\bar{L} + \bar{K}_{nt} \bar{V})X_{nt}\} / \bar{M}_{nt}$$

$$Y_{nt} = \bar{K}_{nt} X_{nt}$$

(v) Total condenser:

$$D = V - L$$

$$\dot{X}_D = \{\bar{V}(Y_{nt} - X_D)\} / \bar{M}_D$$

Note:

$$\bar{K}_i = \frac{\alpha \bar{x}_i}{[1 + (\alpha - 1)\bar{x}_i]^2}$$

APPENDIX B

Basic Operations for Qualitative-model Simplification: ENVISION Arithmetic

Two operations are useful for model simplification.

(i) Direct substitution

can be simplified to

Consider the following confluences

$$[x] = [y] \quad (C5)$$

$$[x] = [y] \quad (C1)$$

$$[y] = [z]. \quad (C2)$$

A straightforward way to simplify the equations is by substituting (C2) into (C1). Therefore, we have

$$[x] = [z]. \quad (C3)$$

and possesses the same qualitative description.

Proof. Since (C4) is the sufficient condition for (C5), this can be proved by simply examining the patterns of $[x]$ and $[y]$ which satisfy (C4).

Another operation of interest is an obvious one. The confluence

$$[x] - [y] + [y] \quad (C6)$$

(ii) Self-elimination**Theorem.** The following confluence

can be simplified into

$$[x] = [x] + [y] \quad (C4)$$

$$[x] = [y]. \quad (C7)$$

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