Complementarity Formulation for the Representation of Algebraic Systems Containing Conditional Equations

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Abstract: Conditional models arise in chemical engineering when modeling systems involve physicochemical discontinuities, such as phase transitions. Zaher (1993) and Grossmann and Turkay (1996) show that one can represent conditional models as an algebraic system of disjunctive equations. This work proposes a new complementarity formulation for the representation of algebraic systems of disjunctive equations. This formulation not only establishes the complementarity condition among equations belonging to different disjunctive terms but also enforces simultaneous satisfaction of all of the equations in the same disjunctive term. This approach represents an alternative to MILP formulations, avoiding discrete decisions; it also avoids the need for special procedural nonlinear techniques as required by the boundary crossing algorithm (Zaher, 1991). We identify the disadvantages associated with the proposed formulation. Solving the resulting nonlinear system of equations relies on the assumption of nondegeneracy of the solution to the complementarity equations. The proposed complementarity representation performed reliably on several example problems where the number of equations in each disjunctive term is small.

Keywords: Conditional models, algebraic system of disjunctive equations, complementarity formulation.

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1 INTRODUCTION

The design and simulation of engineering processes require one to find the solution to a large system of linear and/or nonlinear equations. This work is particularly concerned with the solution of conditional models. Conditional models exist when the defining equations of the system depend on where the model solution lies. A conditional model consists of a system of equations expressed by two sets: a globally defined invariant set of equations and a variant (or locally defined) set of conditional equations which are expressed as disjunctions. Zaher(1993) and Grossmann and Turkay (1996) have already shown that this problem reduces to representing and finding the solution to the system of disjunctive equations:

$$\begin{aligned} &\underline{h}(\underline{x}) = 0 \\ &\bigvee_{i \in D_k} \begin{bmatrix} r^i_{jk}(\underline{x}) = 0 \\ g^i_{lk}(\underline{x}) \le 0 \end{bmatrix} \quad k \in K \qquad \begin{matrix} \forall j \in [1 \ldots \beta_k] \\ \forall l \in [1 \ldots \gamma_k] \end{matrix} \\ &x \in R^n \end{aligned} \tag{1}$$

where $\underline{h}(\underline{x})$ and $\underline{r}^i_k(\underline{x})$ represent the invariant and the variant sets of equations respectively, K represents the set of disjunctions and the index i is used to indicate the i-th term in each disjunction D_k. The vector $\underline{h}(\underline{x})$ is m-dimensional, and it is assumed that $\underline{r}^i_k(\underline{x})$ is β_k-dimensional and that $\underline{g}^i_k(\underline{x})$ is γ_k-dimensional, for all i in D_k. The equations $\underline{h}(\underline{x})$ can be said to be defined over the entire feasible region, while the inequalities $\underline{g}^i_k(\underline{x})$ define the domain of validity of each variant set of equations $\underline{r}^i_k(\underline{x})$. In that way, each variant set of equations is confined to some subregion resulting from the dissection of the feasible region (Zaher, 1991). The solution to the system will be given by the vector $\hat{\underline{x}}$ satisfying the invariant set $\underline{h}(\underline{x})$ and exactly one set of equations for each of the disjunctions, providing that the corresponding set of inequalities is satisfied. Grossmann and Turkay (1996) addresses the existence and uniqueness of the solution for the linear case. Similarly, for the nonlinear case, we may establish that there exists a unique solution $\hat{\underline{x}}$ to (1), if all but one term in each disjunction cannot be satisfied, that is:

$$g^i_{lk}(\underline{x}^i) > 0 \quad \text{for} \quad \underline{h}(\underline{x}^i) = 0, \quad r^i_{jk}(\underline{x}^i) = 0 \qquad \forall i \ne \hat{i}, \; k \in K, \; j \in [1 \ldots \beta_k], \; l \in [1 \ldots \gamma_k]$$

Fluid transition represents the example of a conditional model commonly encountered in chemical engineering. Figure 1, taken from the work of Zaher (1995), illustrates. In this case, we must incorporate alternative equations for the transport properties and velocity bounds within the model, using the simultaneously calculated value of the flow type indicator (Reynolds or Mach number) relative to some critical value to determine which is active.

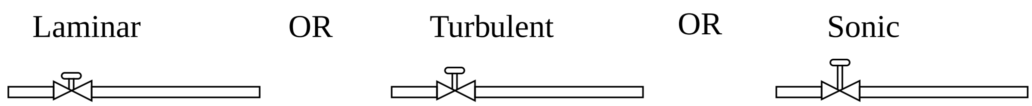

FIGURE 1 Fluid flow transition

It is important to recognize that modeling is a user dependent task. Frequently, different modelers produce different formulation for the same problem and, as a consequence, different approaches and techniques may be used to find a solution to it. One can formulate conditional models as mixed-integer programming problems. See for example Grossmann and Turkay (1996). Besides the mixed-integer formulation, some alternative approaches exist which, in principle, could avoid the need for discrete decisions. Zaher (1991) proposed one of this approaches with the boundary crossing algorithm. This work, however, focuses on a second approach, the complementarity representation of conditional models.

1.1 COMPLEMENTARITY APPROACH

Over the last thirty years, the class of problems known as complementarity problems has become increasingly popular as a tool for addressing practical problems arising in mathematical programming, economics, engineering, and the sciences (Billups, 1995; Ferris and Pang, 1995). Several works have documented the basic theory, algorithms and applications of complementarity problems. Dirske and Ferris (1995) give examples of how to formulate many popular problems as mixed complementarity problems (MCP). Billups (1995) describes the standard forms for the different classes of complementarity problems and proposes strategies which enhances the robustness of Newton-based methods for solving these problems. More (1994) formulates the complementarity problem as a nonlinear least square problem and gives convergence properties for his approach. In this work, we describe an extension to the standard complementarity formulation (Billups, 1995) for the representation of conditional models.

2 PROBLEM FORMULATION

In general, the nonlinear complementarity problem is expressed as the following set of equations and inequality constraints:

$$\underline{x}^T \cdot \underline{r}(\underline{x}) = 0$$
$$\underline{x} \geq 0 \qquad \underline{r}(\underline{x}) \geq 0 \tag{2}$$

There is certain lack of symmetry in the previous formulation. One of the functions is quite arbitrary while the other is the vector of variables. Many commonly occurring problems have a more general form:

$$\underline{r}^1(\underline{x})^T \cdot \underline{r}^2(\underline{x}) = 0 \tag{3}$$

which is called the vertical nonlinear complementarity problem (Ferris and Pang, 1995). It is possible, of course, to have more than two vectors of functions in the above equations:

$$\underline{r}^1(\underline{x}) \cdot \underline{r}^2(\underline{x}) \ldots \underline{r}^k(\underline{x}) = 0$$
$$\underline{r}^i(\underline{x}) \geq 0 \qquad \forall i \in [1 \ldots k] \tag{4}$$

For the case of a *single conditional equation* in a disjunctive statement, Zaher,(1995) show that there exits an equivalent representation by using a standard complementarity formulation as follows:

$$\begin{bmatrix} r_i + g_i(\underline{x}) < 0 \\ r_i = 0 \end{bmatrix} \vee \begin{bmatrix} r_i + g_i(\underline{x}) \geq 0 \\ g_i(\underline{x}) = 0 \end{bmatrix} \quad \Longleftrightarrow \quad \begin{matrix} r_i \cdot g_i(\underline{x}) = 0 \\ r_i \geq 0 \qquad g_i(\underline{x}) \leq 0 \end{matrix} \tag{5}$$

A typical example of this equivalence can be found while representing the complementarity equations arising from the Karush-Kuhn-Tucker conditions of an optimization problem. There are also cases in which physicochemical transitions are complementary in nature and can be represented by such a formulation. For instance, Zaher (1995) represents the adiabatic compressible flow in a disjunctive statement with an equivalent complementarity representation:

$$\begin{bmatrix} P_d - P_f < M_f - 1 \\ M_f - 1 = 0 \end{bmatrix} \vee \begin{bmatrix} P_d - P_f \geq M_f - 1 \\ P_d - P_f = 0 \end{bmatrix} \Longleftrightarrow \begin{matrix} (M_f - 1) \cdot (P_d - P_f) = 0 \\ M_f \leq 1 \qquad P_f \geq P_d \end{matrix} \tag{6}$$

On the other hand, if the disjunctive statement has *more than one equation in each disjunctive term*, as the example of the heat exchanger given also by Zaher (1995), the standard complementarity formulation is not equivalent to the disjunctive representation:

$$\begin{bmatrix} \sum_{i \in C} x_i^2 + \phi^1 < 1 \\ \phi^1 = 0 \\ \eta^2 = 0.5 \end{bmatrix} \vee \begin{bmatrix} \sum_{i \in C} x_i^2 + \phi^1 \geq 1 \\ \sum_{i \in C} x_i^2 = 1 \\ \eta^1 = 0.5 \end{bmatrix} \not\Longleftrightarrow \begin{matrix} \phi^1 \cdot \left(\sum_{i \in C} x_i^2 - 1 \right) = 0 \\ (\eta^2 - 0.5) \cdot (\eta^1 - 0.5) = 0 \\ \phi^1 \geq 0 \qquad \sum_{i \in C} x_i^2 \leq 1 \end{matrix} \tag{7}$$

Notice that in the disjunctive representation all the equations belonging to the same disjunctive term have to be satisfied simultaneously, a restriction which is not represented by the standard complementarity formulation. In the following section, we propose the representation of disjunctive sets of algebraic equations as a complementarity problem. The formulation described in this paper not only establishes the complementarity condition among alternative sets of equations, but it also enforces simultaneous satisfaction of all the equations in the solution set. It is important to mention that we are aware of many disadvantages associated with this representation, but our motivation relies on the fact that a complementarity formulation only requires the solution of one square system of nonlinear equations, avoiding all of the complications encountered in procedural techniques such as the boundary crossing algorithm (Zaher, 1991) and the discrete decision making of an MINLP solution. Before going further in the description of our approach, in Figure 2 we explain the relevant terminology employed in this paper.

2.1 COMPLEMENTARITY REPRESENTATION OF A CONDITIONAL MODEL

As in most of the complementarity approaches reported in the literature, in this paper we assume the nondegeneracy of the solution to the complementarity problem. With this assumption we leave out all those cases in which equations belonging to different terms of the same disjunctive statement are simultaneously satisfied. In addition, we will assume that the nonlinear problem can be represented by a function $\underline{r}(\underline{x})\mathbf{:}\boldsymbol{R}^n{}_{+} \longrightarrow \boldsymbol{R}^n$; that is, we assume that we can rearrange the equations so that the residuals of the conditional equations belonging to a non-solution disjunctive term will always be positive.

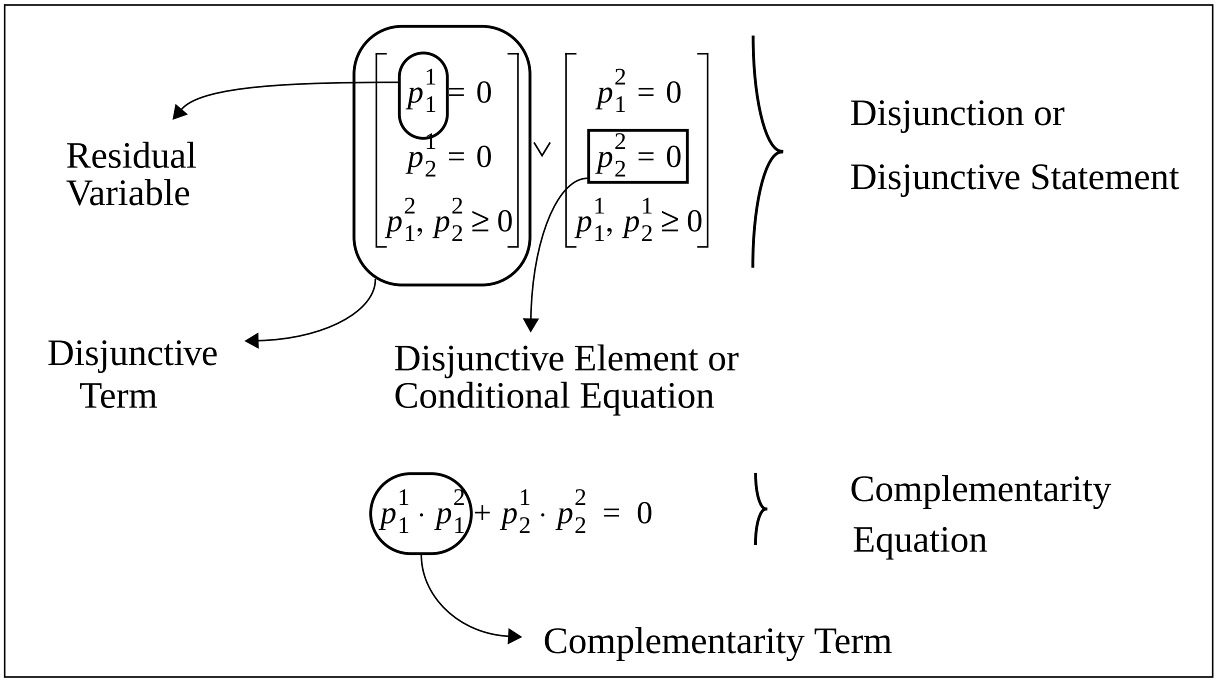

FIGURE 2 Description of our terminology

The formulation presented here is an extension of that presented by More(1994), who reformulates the nonlinear complementarity problem (2) as:

$$\underline{r}(\underline{x}) = \underline{p}$$
$$P \cdot \underline{x} = \underline{0} \qquad (8)$$
$$\underline{x} \geq 0 \qquad \underline{p} \geq 0$$

where P is the diagonal matrix diag(p_i).

For the purpose of illustration, consider the example of the heat exchanger given by (7).

Defining positive residuals p_j^i for each of the equations:

$$\phi^1 = p_1^1 \qquad 1 - \sum_{i \in C} x_i^2 = p_1^2$$
$$\eta^2 - 0.5 = p_2^1 \qquad 0.5 - \eta^1 = p_2^2 \tag{9}$$

Representing the disjunctive statement in terms of those residuals:

$$\begin{bmatrix} p_1^1 = 0 \\ p_2^1 = 0 \\ p_1^2, p_2^2 \geq 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_2^2 = 0 \\ p_1^1, p_2^1 \geq 0 \end{bmatrix} \tag{10}$$

Notice that we have been arranged the conditional equations in (9) in such a way that all the variables p_j^i are always positive. In order to do that, we used the physical insight given by the nature of the problem. In term of the residuals, the standard complementarity formulation is given by:

$$p_1^1 \cdot p_1^2 = 0$$
$$p_2^1 \cdot p_2^2 = 0 \tag{11}$$
$$p_j^i \geq 0 \qquad i \in [1\ldots2] \qquad j \in [1\ldots2]$$

The disjunctive statement requires either both p_1^1 and p_2^1 or both p_1^2 and p_2^2 simultaneously to be zero. That is not a restriction included in the standard complementarity formulation (11). We propose the following formulation to represent the disjunctive statement instead:

$$p_1^1 \cdot p_1^2 + p_2^1 \cdot p_2^2 = 0$$
$$p_1^1 \cdot p_2^2 + p_2^1 \cdot p_1^2 = 0 \tag{12}$$
$$p_j^i \geq 0 \qquad i \in [1\ldots2] \qquad j \in [1\ldots2]$$

Since the residuals are all positive, the set of equations in (12) not only contains the complementarity condition given by the standard representation (11) but also enforces the simultaneous satisfaction of all the equations defined in the same terms of the disjunction. Also, it is important to realize that the inequality constraints in (12) are only bounds in the residual variables, and we can use them to guide our search for a solution to the resulting square system of equations:

- The original disjunctive statement provides 2 equations in either of its cases.
- The complementarity formulation provides 6 equations but introduces 4 new variables, also a net of 2 equations.

For cases in which the domain of validity is given by inequality constraints, we reformulate the problem by adding two slacks to the inequality and express the complementarity condition between these slack variables. Consider for example the laminar-turbulent flow transition given by:

$$\begin{bmatrix} Re = 64/f \\ Re \le 2100 \end{bmatrix} \vee \begin{bmatrix} Re = (0.206307/f)^4 \\ Re \ge 2100 \end{bmatrix} \tag{13}$$

If we define residuals for the equalities and slack variables for the inequalities:

$$\begin{gathered} Re - 64/f = p_1^1 \qquad Re - (0.206307/f)^4 = p_1^2 \\ Re = 2100 + p_2^1 - p_2^2 \end{gathered} \tag{14}$$

then the disjunctive statement in terms of residuals and slacks and, therefore, the complementarity equations, are exactly the same as those given in the previous example. Notice that the inequalities become an active part of the system of equations. Also, one of the complementarity equations contains a complementarity product between the two slacks in the inequality, a requirement to avoid multiple solutions.

The result of applying our formulation is a square system of nonlinear equations (including complementarity equations) subject to the positiveness of the slacks and residual variables.

The proposed complementarity representation has the following properties:

1. The number of complementarity equations is equal to the number of equations in each term of

the disjunction to maintain the same number of degrees of freedom as in the original problem.

2. Every residual is multiplied by every residual in all of the other terms of the disjunction. Thus, we will ensure the simultaneous satisfaction of all the equations in the disjunctive term corresponding to the solution and, as a consequence, avoid spurious solutions to the problem.

3. In the example, there are several ways in which we could have accommodated the four complementarity terms in the two complementarity equations. The way in which we have distributed the bilinear terms over the complementarity equations is intended to decrease the possibility of having numerical singularities in the Jacobian of the system while using an iterative scheme based on Newton and quasi-Newton methods. We must avoid having two residual variables from the same disjunctive term being multiplied in two complementarity equations by the same set of residual variables from another disjunctive term. Examine Figure 3. We show a set of complementarity equations and the rows of the Jacobian corresponding to those equations. Note that the equations in Figure 3 contain the same four complementarity terms as the formulation given by (12), but they are grouped differently. In the case presented, if the solution to the problem is $p_1^2 = p_2^2 = 0$, rows 1 and 2 of the Jacobian become numerically dependent as the Newton method approaches the solution. If $p_1^2 + p_2^2 \sim 0$, we could get row 2 multiplying row 1 by the factor p_2^1 / p_1^1. This is not the case for the complementarity equations given by (12).

$$\begin{matrix} p_1^1 \cdot p_1^2 + p_1^1 \cdot p_2^2 = 0 \\ p_2^1 \cdot p_1^2 + p_2^1 \cdot p_2^2 = 0 \end{matrix} \Rightarrow \begin{matrix} p_1^1 \cdot (p_1^2 + p_2^2) = 0 \\ p_2^1 \cdot (p_1^2 + p_2^2) = 0 \end{matrix}$$

	p_1^1	p_1^2	p_2^1	p_2^2
1	$p_1^2 + p_2^2$	p_1^1	0	p_1^1
2	0	p_2^1	$p_1^2 + p_2^2$	p_2^1

FIGURE 3 Numerical singularities in complementarity equations

In the following sections, we formally describe how to obtain a complementarity formulation including all of the properties outlined above. While showing how to generate the complementarity equations, we first consider the case in which the disjunctive statement contains two terms and then we extend the analysis to any number of disjunctive terms.

2.1.1 Representing the Disjunctive Statements in terms of Positive Residual or Slack Variables

Before generating the set of complementarity equations, it is necessary to define positive residual variables (or slack variables for inequalities) for the conditional equations and to represent the disjunctive statements in terms of these positive variables. This task has to be accomplished disregarding the number of terms in each disjunctive statement. As a matter of fact, one of our assumptions here is that the system of equations can be rearranged to obtain this representation. For instance, for the simplest case of one disjunction with two terms (the index k is omitted for simplicity), given the disjunctive set of algebraic equations:

$$\underline{h}(\underline{x}) = 0$$

$$\begin{bmatrix} r_j^1(\underline{x}) = 0 \\ g_l(\underline{x}) \le 0 \end{bmatrix} \vee \begin{bmatrix} r_j^2(\underline{x}) = 0 \\ g_l(\underline{x}) \ge 0 \end{bmatrix} \qquad \begin{matrix} \forall j \in [1 \ldots \beta] \\ \forall l \in [1 \ldots \gamma] \end{matrix} \qquad (15)$$

we reformulate the problem as:

$$\begin{gathered} \underline{h}(\underline{x}) = 0 \\ r_j^1(\underline{x}) - p_j^1 = 0 \\ r_j^2(\underline{x}) - p_j^2 = 0 \qquad \forall j \in [1 \ldots \beta] \quad l \in [\beta + 1 \ldots \beta + \gamma] \\ g_l(\underline{x}) - p_l^1 + p_l^2 = 0 \\ \begin{bmatrix} p_q^1 = 0 \\ p_q^2 \ge 0 \end{bmatrix} \vee \begin{bmatrix} p_q^2 = 0 \\ p_q^1 \ge 0 \end{bmatrix} \quad \forall q \in [1 \ldots \beta + \gamma] \end{gathered} \qquad (16)$$

2.1.2 2-Term Disjunctive Statements

Given the disjunctive statement in terms of the positive residual variables p_q^i, we obtain the set of complementarity equations by using the following:

$$\begin{bmatrix} p_q^1 = 0 \\ p_q^2 \geq 0 \end{bmatrix} \vee \begin{bmatrix} p_q^2 = 0 \\ p_q^1 \geq 0 \end{bmatrix} \quad \forall q \in [1 \ldots \beta + \gamma]$$

$$\Updownarrow$$

$$\sum_{t=1}^{\beta+\gamma-s} p_t^1 \cdot p_{t+s}^2 + \sum_{t=\beta+\gamma-s+1}^{\beta+\gamma} p_t^1 \cdot p_{t+s-\beta-\gamma}^2 = 0 \qquad \forall s \in [0 \ldots \beta + \gamma - 1]$$

$$p_q^i \geq 0 \qquad \forall i \in [1 \ldots 2],\ q \in [1 \ldots \beta + \gamma] \tag{17}$$

Hence, the resulting nonlinear system of equations is:

$$\underline{h}(\underline{x}) = 0$$

$$r_j^1(\underline{x}) - p_j^1 = 0$$

$$r_j^2(\underline{x}) - p_j^2 = 0 \qquad \forall j \in [1 \ldots \beta],\ l \in [\beta + 1 \ldots \beta + \gamma]$$

$$g_l(\underline{x}) - p_l^1 + p_l^2 = 0 \tag{18}$$

$$\sum_{t=1}^{\beta+\gamma-s} p_t^1 \cdot p_{t+s}^2 + \sum_{t=\beta+\gamma-s+1}^{\beta+\gamma} p_t^1 \cdot p_{t+s-\beta-\gamma}^2 = 0 \qquad \forall s \in [0 \ldots \beta + \gamma - 1]$$

$$p_q^i \geq 0 \qquad \forall i \in [1 \ldots 2],\ q \in [1 \ldots \beta + \gamma]$$

Note that, not taking in account the bounds in the residual variables, the resulting nonlinear system of equations is square.

The generation of the complementarity equations given by (17) is illustrated in Figure 4. Basically, in a complementarity equation each residual variable of one disjunctive term is multiplied by one residual variable of the other disjunctive term, and, for successive complementarity equations, the order of the residual variables in the second term is successively shifted by one.

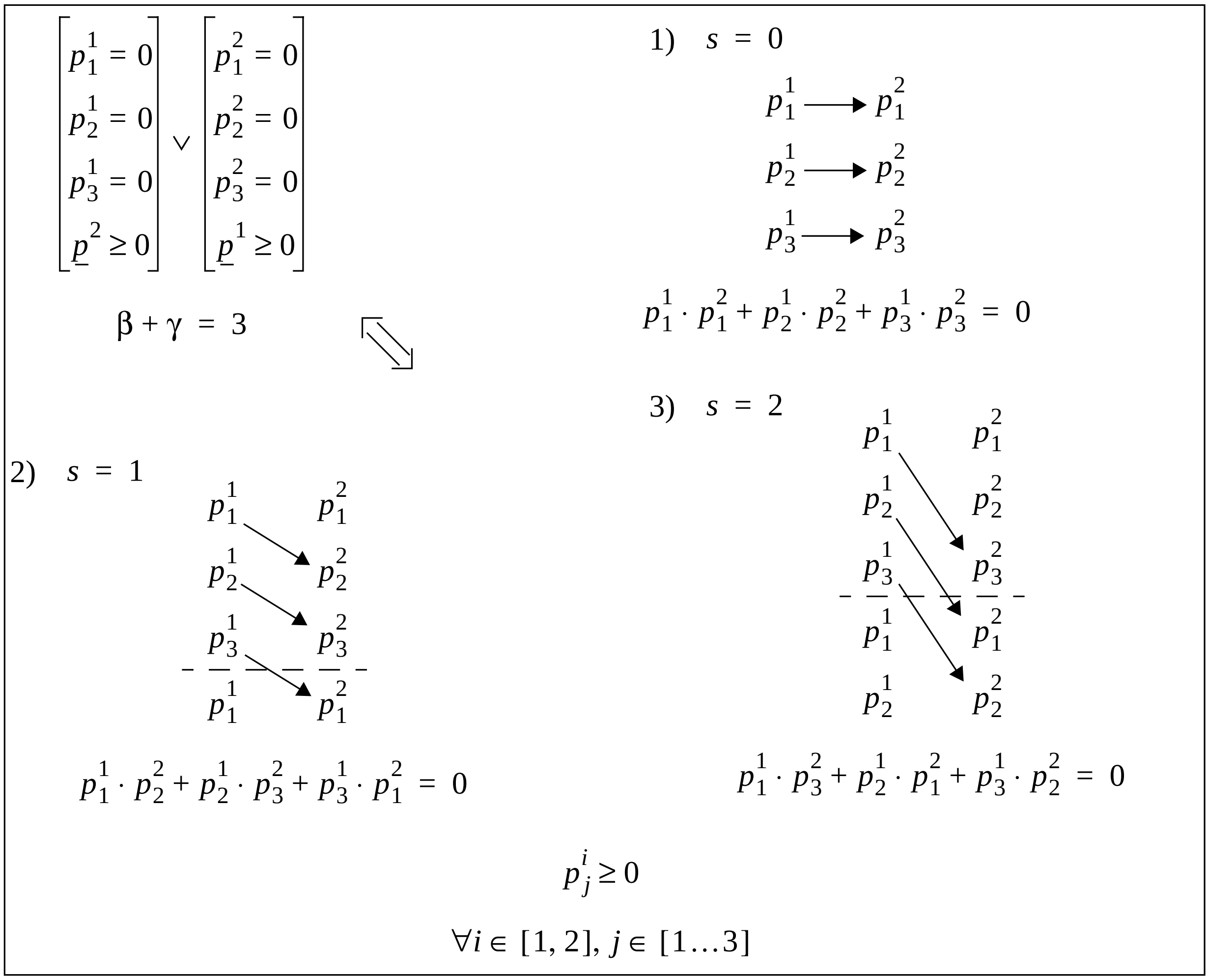

FIGURE 4 Generation of complementarity equations in a two-term disjunction.

Every possible complementarity term resulting from the multiplication of positive residual variables belonging to different disjunctive terms is included in complementarity equations (17). This feature ensures that, in order to satisfy the complementarity equations, all the residual variables of at least one disjunctive term have to be simultaneously zero. The proof is simple. Assume that, in each of the disjunctive terms, there is only one nonzero residual variable. Since all of the possible complementarity terms exist in the complementarity equations, a complementarity term containing those residual variables must exist. Find the complementarity term that contains just these nonzero residual variables. Since the product of those variables will be nonnegative, that term will force the complementarity equation in which it exists to be greater than zero, i.e., it will not be satisfied. To be satisfied, at least one of the residual variables i the complementarity term must be zero, contradicting our original assumption. Thus, in order to satisfy the complementarity equations, at least one disjunctive term must have all its residual variables equal to zero. In other words, a complete set of conditional equations in at least one of the disjunctive terms will be simultaneously satisfied.

As a consequence of the previous analysis, if the complete set of nonlinear equations (including the complementarity equations) is satisfied, then the solution vector $\hat{x}$ will correspond to a consistent solution to the conditional model. Moreover, if we assume uniqueness of the solution, then the vector $\hat{x}$ will be the unique solution to the conditional model.

Another property of the complementarity set of equations given by (17) is that, in every complementarity equation, all the residual variables are incident, and each of them is incident only once. That is intended to decrease the possibility of having numerical singularities in the Jacobian of the system as explained before. In fact, by analyzing the Jacobian of the formulation (17) under the assumption of nondegeneracy of the solution, it can be shown that the possibility of having numerical singularities is eliminated. If nondegeneracy occurs, the residuals in the equations of the disjunctive set not corresponding to the solution are expected to be different from zero, and, therefore, they will provide a pivot in the jacobian matrix for all the complementarity equations (note that the number of positive residuals is equal to the number of complementarity equations).

2.1.3 Generalization to any number of terms in the Disjunctive Statement

When the disjunctions contain more than two terms, we generate the complementarity equations by applying recursively the same equation given in (17). We assume again that we can obtain a disjunctive statement in terms of positive residual variables. Consider the following simple example of a disjunction with three terms:

$$\begin{bmatrix} p_1^1 = 0 \\ p_2^1 = 0 \\ \underline{p}^2, \underline{p}^3 \geq 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_2^2 = 0 \\ \underline{p}^1, \underline{p}^3 \geq 0 \end{bmatrix} \vee \begin{bmatrix} p_1^3 = 0 \\ p_2^3 = 0 \\ \underline{p}^1, \underline{p}^2 \geq 0 \end{bmatrix} \tag{19}$$

We apply equation (17) to the first two disjunctive terms:

$$\left[\begin{bmatrix} p_1^1 = 0 \\ p_2^1 = 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_2^2 = 0 \end{bmatrix}\right] \vee \begin{bmatrix} p_1^3 = 0 \\ p_2^3 = 0 \end{bmatrix}$$

$$\Updownarrow \qquad p_j^i \geq 0 \quad \forall i \in [1\ldots3],\ j \in [1\ldots2]$$

$$\begin{bmatrix} p_1^1 \cdot p_1^2 + p_2^1 \cdot p_2^2 = 0 \\ p_1^1 \cdot p_2^2 + p_2^1 \cdot p_1^2 = 0 \end{bmatrix} \vee \begin{bmatrix} p_1^3 = 0 \\ p_2^3 = 0 \end{bmatrix} \tag{20}$$

and do it again for the resulting two-term disjunction:

$$\begin{gathered} (p_1^1 \cdot p_1^2 + p_2^1 \cdot p_2^2) \cdot p_1^3 + (p_1^1 \cdot p_2^2 + p_2^1 \cdot p_1^2) \cdot p_2^3 = 0 \\ (p_1^1 \cdot p_1^2 + p_2^1 \cdot p_2^2) \cdot p_2^3 + (p_1^1 \cdot p_2^2 + p_2^1 \cdot p_1^2) \cdot p_1^3 = 0 \\ p_j^i \geq 0 \quad \forall i \in [1\ldots3],\ j \in [1\ldots2] \end{gathered} \tag{21}$$

A complementarity set of equations obtained in this form still will include the properties outlined before for a two-term disjunction:

1. It will result in a square system of equations.
2. In order to satisfy the complementarity equations, all the equations of at least one set of conditional equations have to be simultaneously satisfied.
3. Under the assumption of nondegeneracy, the Jacobian of the system of equations can be shown to be nonsingular.

The reasoning employed to prove the previous statements is the same as that in the case of a two-term disjunction discussed above.

2.1.4 About the Complementarity Formulation

The complementarity formulation is not without problems:

1. First of all, the problem grows quickly. If (β+γ) is the number of equations in each term of the

disjunction and D is the number of terms in the disjunction, the number of equations representing the disjunctive statement in the complementarity formulation is $(\beta+\gamma)(D+1)$. That number includes both the complementarity equations and the equations defining the positive residual variables.

2. The number of bilinear terms (or terms including products among variables) incorporated in each equation also grows with the number of equations in each term of the disjunction. The combinatorial nature of the problem is encapsulated here.
3. The performance of optimization techniques is badly affected by the introduction of nonconvexities (multiplication among variables) to the system of equations.
4. Numerical singularities still arise for cases in which the solution resides on a boundary. That is the main reason for the assumption of nondegeneracy.

In general, we are presenting this approach as a very favorable alternative when the number of equations in each disjunctive term is small.

3 ILLUSTRATIVE EXAMPLES

We have represented and solved several examples of algebraic systems of disjunctive equations found in the literature by using a complementarity formulation. Appendix A presents the complementarity equations (or a representative part of them) for each of those examples.

In examples 1 through 4 the disjunctive statements contain only two terms, and we generated the complementarity equations by strictly using the formulation proposed in (17). In his work, Zaher (1995) solved examples 1 and 3 as optimization problems, by defining an objective function and an appropriate selection of the degrees of freedom. In this work we solve examples 1 and 3 as simulation problems by specifying fixed values to the appropriate variables (free variables in the optimization) and removing the objective function. We could use the complementarity formulation for an optimization scheme, but at this time we wanted to avoid the separated issue of handling the optimization of a system containing bilinearities.

The degree of complexity increases in examples 5 and 6 since the disjunctive statements contain three terms. In those cases, we added two slacks to the conditional equations in one of the disjunctive terms which will allow some of the conditional equations to have a negative residual.

In examples 5 and 6 we do not use the general formulation proposed for three-term disjunctions. Instead, we use those examples to show how sometimes the specific structure of the disjunctive statement can be used to simplify the resulting system of complementarity equations.

Where reported, the initial values for the variables are the same as those given in the reference. To solve the examples, we used our ASCEND solver which applies the modified Levenberg-Marquardt algorithm given in Westerberg and Director (1979). This method is preferred because it is a least squares solver which may help to overcome the numerical singularities arising from the complementarity formulation. In all the cases the solution of only one nonlinear system of equations is required. Also, in all the examples the number of equations in each disjunctive term is very small, and, as a consequence, the complexity of the equations involving products among slack variables is not as bad as can be expected with problems of larger size.

EXAMPLE 1 Fluid Transition (Zaher, 1995).

This example describes the flow of a compressible gas in an adiabatic frictional circular pipe of constant diameter. Nonsmooth functionality occurs due to the possible transition between sonic-not sonic flow at the outlet of the pipe. It corresponds to a simplest case of a conditional model: the problem contains only one disjunction with only one equation in each term. The alternatives for the solution of the problem are represented by:

$$\begin{bmatrix} P_d - P_f < M_f - 1 \\ M_f - 1 = 0 \end{bmatrix} \vee \begin{bmatrix} P_d - P_f \geq M_f - 1 \\ P_d - P_f = 0 \end{bmatrix}$$

in which one of the terms corresponds to sonic flow (Match number $M_f=1$) and the other to not sonic flow ($P_d=P_f$). The equations describing the thermodynamics are omitted for simplicity and can be found in Zaher (1995).

As we already mentioned, Zaher (1995) reported the solution to this problem as an optimization problem. We run simulations for values of the diameter of the pipe between 2 cm and 9 cm, such that we could make sure that both of the alternative cases are reached by using the complementarity representation.

EXAMPLE 2 Phase Equilibria (Zaher, 1995).

An isothermal flash is applied to a ternary system involving benzene, ethanol and water. According to the phase diagram of this mixture and, depending on the values of pressure and temperature, three phases can be expected to exist simultaneously, an aqueous liquid phase, an organic liquid phase, and a vapor phase. The existence or nonexistence of each phase can be represented as a conditional statement. For instance, to represent the existence of the aqueous phase, the following statement applies:

$$\begin{bmatrix} \sum_{i \in C} y_i^A + \phi^A < 1 \\ \phi^A = 0 \end{bmatrix} \vee \begin{bmatrix} \sum_{i \in C} y_i^A + \phi^A \geq 1 \\ \sum_{i \in C} y_i^A = 1 \end{bmatrix}$$

as obtained by Michelsen (1982) and Zaher(1995). Since there are three possible phases, we require three similar disjunctions to represent the behavior. There are only one equation in each disjunction though and, therefore, only one complementarity equation for each of them is required.

EXAMPLE 3 Heat Exchanger (Zaher, 1995).

A very detailed explanation of this example can be found in Zaher (1995). It represents a case in which a conditional model contains differential equations that have to be integrated. The approach suggested is to discretize the differential equations and treat the problem as a conditional model with only algebraic equations. To accomplish this, Zaher (1995) introduced a relay method: the point in the domain of integration where transition occurs is continuously passed along, as a baton in a relay race, from one element to another by successive contractions and expansions of the individual elements. Switching stations at which the analogous baton transfer occurs must first be positioned. This example is introduced in Figure 5. Three finite elements are chosen with one switching station. To outline the three elements, four positions referenced by the indices {0...3} are used. The domain of integration is transformed to the dimensionless variable η which varies from zero to one. The difficulty with this model is that, in addition to solving for the temperature profile, the dimension of the finite elements are to be solved for as well.

Zaher (1995) shows that the three cases shown in Figure 5 can be represented as a conditional model including the following disjunctive statement:

$$\begin{bmatrix} \sum_{i \in C} x_i^0 + \phi^0 < 1 \\ \sum_{i \in C} x_i^2 + \phi^1 < 1 \\ \phi^0 = 0 \\ \eta^1 = 0 \\ \eta^2 = 0.5 \\ \phi^1 = 0 \end{bmatrix} \vee \begin{bmatrix} \sum_{i \in C} x_i^0 + \phi^0 \geq 1 \\ \sum_{i \in C} x_i^2 + \phi^1 < 1 \\ \sum_{i \in C} x_i^0 = 1 \\ \sum_{i \in C} x_i^1 = 1 \\ \eta^2 = 0.5 \\ \phi^1 = 0 \end{bmatrix} \vee \begin{bmatrix} \sum_{i \in C} x_i^0 + \phi^0 \geq 1 \\ \sum_{i \in C} x_i^2 + \phi^1 \geq 1 \\ \sum_{i \in C} x_i^0 = 1 \\ \sum_{i \in C} x_i^1 = 1 \\ \eta^1 = 0.5 \\ \sum_{i \in C} x_i^2 = 1 \end{bmatrix}$$

where ϕ represents the fraction of the hot stream which is condensed and x is a vector representing the composition of the condensation droplets.

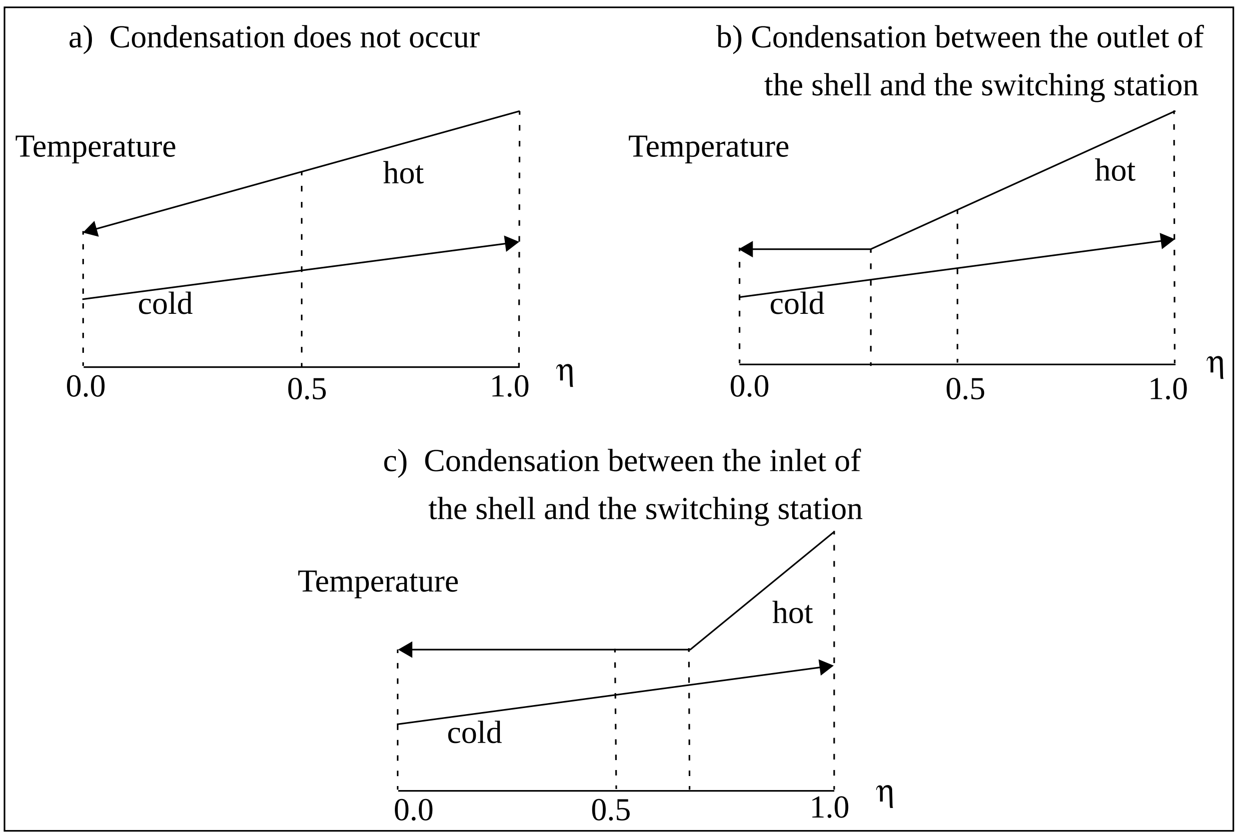

FIGURE 5 Alternative heat exchanger temperature profiles.

In order to obtain an equivalent complementarity formulation, we start by recognizing that we can decouple the previous disjunctive statement in two independent disjunctions:

$$\begin{bmatrix} \phi^0 = 0 \\ \eta^1 = 0 \\ \sum_{i \in C} x_i^{\,0} + \phi^0 < 1 \end{bmatrix} \vee \begin{bmatrix} \sum_{i \in C} x_i^{\,0} = 1 \\ \sum_{i \in C} x_i^{\,1} = 1 \\ \sum_{i \in C} x_i^{\,0} + \phi^0 \geq 1 \end{bmatrix}$$

and

$$\begin{bmatrix} \phi^1 = 0 \\ \eta^2 = 0.5 \\ \sum_{i \in C} x_i^{\,2} + \phi^1 < 1 \end{bmatrix} \vee \begin{bmatrix} \sum_{i \in C} x_i^{\,2} = 1 \\ \eta^1 = 0.5 \\ \sum_{i \in C} x_i^{\,2} + \phi^1 \geq 1 \end{bmatrix}$$

We run simulations for values of area between 250 ft^2 and 1104 ft^2 and values of flowrates between 250 lbmole/hr and 380 lbmole/hr, ranges analyzed by Zaher while finding an optimal solution.

EXAMPLE 4 Pipeline Network (Bullard and Biegler, 1992)

Consider the pipe network shown in Figure 6 solved previously by Bullard and Biegler (1992). This problem can be described by the system of equations:

$$\sum_j Q_{ij} + \sum_j Q_{ji} = w_i \qquad \forall node\ i$$

$$H_{ij} = K \cdot sign(Q_{ij}) \cdot Q_{ij}^{\,2} \qquad \forall arc\ ij\ without\ valve$$

$$\begin{bmatrix} K \cdot Q_{ij}^{\,2} = 0 \\ H_{ij} \leq 0 \end{bmatrix} \vee \begin{bmatrix} K \cdot Q_{ij}^{\,2} = H_{ij} \\ H_{ij} \geq 0 \end{bmatrix} \qquad \forall arc\ ij\ with\ valve$$

$$H_{ij} = P_i - P_j \qquad \forall arc\ ij$$

$$Q_{ij} \geq 0 \qquad \forall arc\ ij\ with\ valve$$

The first equation is a flow balance around each node, the second is the Hazen-Williams relation for pipes with no valve, and the third is the relation between pressure drop and flowrate. Notice that an equivalent disjunctive representation for the Hazen-Williams relations can be given by :

$$\begin{bmatrix} H_{ij} = -K \cdot Q_{ij}^{2} \\ Q_{ij} \le 0 \end{bmatrix} \vee \begin{bmatrix} H_{ij} = K \cdot Q_{ij}^{2} \\ Q_{ij} \ge 0 \end{bmatrix} \qquad \forall arc\ ij\ without\ valve$$

All pipes are 100 ft long and 6 in diameter, and the fluid is water: ρ = 62.4/lbm/ft3, μ = 1 cP and ε = 0.01 in. Pressures and inflow/outflow rates specifications are given in Table 1. Rates not specified are equal to zero (except the one in node 17 which is an unknown). Pressures not specified are unknowns in the problem. The starting point and converged flowrates are given in Table 2.

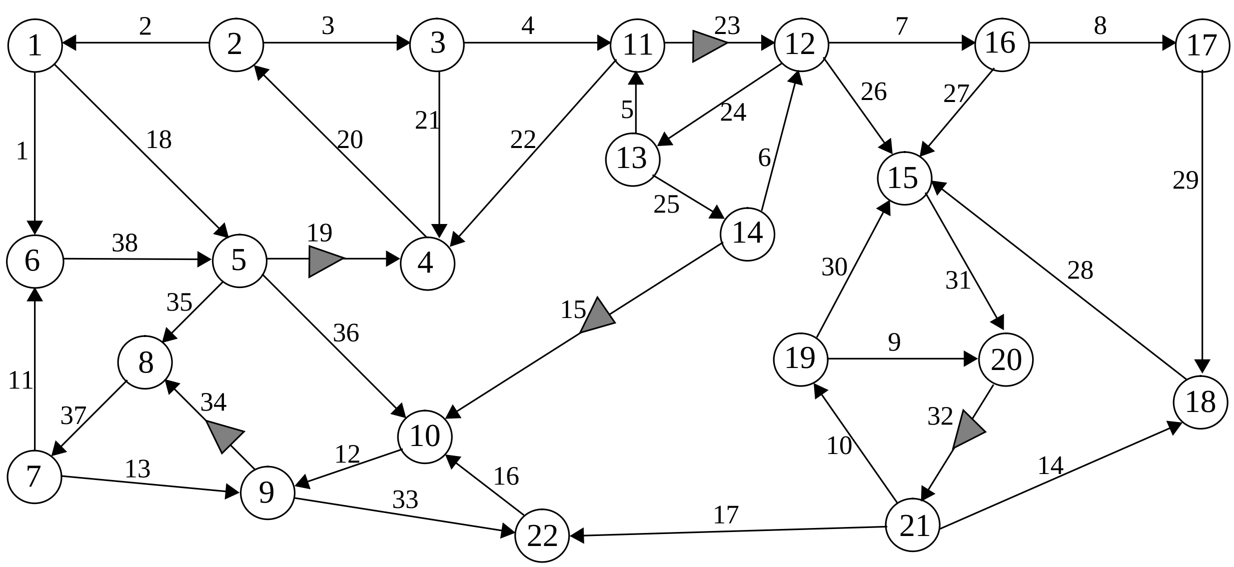

FIGURE 6 Pipe network with five check valves

Table 1: Pressures and inflow/outflow rates for Example 4

Node No.	Pressure P (psig)	Inflow rate w (gpm)
1		897.6
7		1570.9
11		-897.6
17	0	
20		-448.8
22		673.2

EXAMPLE 5 Simple L-V Flash Calculation (King, 1980)

This situation corresponds to a simple equilibrium calculation as given by King (1980). Basically, the problem consists of finding a solution to the well known Rachford-Rice equation:

$$x_i = \frac{z_i}{(K_i - 1) \cdot (V/F) + 1} \qquad y_i = \frac{K_i \cdot z_i}{(K_i - 1) \cdot (V/F) + 1}$$

$$\sum_i y_i - \sum_i x_i = 0 \qquad \Longrightarrow \qquad f(V/F) = \sum_i \frac{z_i \cdot (K_i - 1)}{(K_i - 1) \cdot (V/F) + 1} = 0$$

In the presence of two phases in equilibrium, the iterative calculation involves applying a convergence procedure until a value of V/F is found such that *f(V/F) = 0*. However, it may well happen that the specifications of the problem do not correspond to a system with two phases present. For the case of a Liquid-Vapor equilibrium, King proposes the following criteria to differentiate among the different cases: *f(V/F)* will be positive at V/F=0 and negative at (V/F)=1. Therefore, if *f(V/F)* is negative at V/F=0, the system is subcooled liquid. If *f(V/F)* is positive at V/F=1, the system is superheated vapor. This behavior can be represented in term of the following disjunctive statement:

Table 2: Starting point and converged flowrates for Example 4

Pipe No.	Estimated flow $Q^{(0)}$ (gpm)	Converged flow Q* (gpm)
1	-48.5	-223.345
2	-640.7	-894.840
3	393.2	520.818
4	538.9	883.254
5	-32.3	-435.573
6	490.2	180.240
7	649.2	533.254
8	904.7	877.652
9	112.2	315.876
10	232.5	602.421
11	402.3	541.160
12	-420.4	-229.091
13	687.3	585.972
14	621.7	701.302
15	-719.2	0.0
16	52.7	-273.643
17	1199.0	-1303.723
18	305.4	226.105
19	582.8	943.137
20	-247.5	-374.022
21	-145.7	-362.435
22	-684.6	-954.723
23	293.6	504.804
24	-261.3	-255.153
25	-229.0	180.420
26	-395.1	407.123
27	-254.8	-344.398
28	-268.9	-216.346
29	-890.6	-917.648
30	120.3	286.546
31	-8.1	132.925
32	-344.7	0.0
33	473.1	356.88
34	-206.2	0.0
35	-275.0	-443.768
36	351.5	44.552
37	-481.2	-443.768
38	353.9	317.815

$$\sum_i \frac{z_i \cdot (K_i - 1)}{(K_i - 1) \cdot (V/F) + 1} = R - V/F$$

$$\begin{bmatrix} V/F = 0 \\ R \le 0 \end{bmatrix} \vee \begin{bmatrix} V/F = R \\ 0 \le R \le 1 \end{bmatrix} \vee \begin{bmatrix} V/F = 1 \\ R \ge 1 \end{bmatrix}$$

This disjunction include three disjunctive terms, but a complementarity is still possible. For testing the proposed formulation, we took a mixture 20% of butane, 50% of pentane and 20 % of hexane, at 10 atm, and performed simulations for a broad range of temperatures (150 K to 890 K) to ensure the convergence of the method for the three possible cases.

EXAMPLE 6 Linear Mass Balance (Grossmann and Turkay, 1996)

This example, illustrated in Figure 7, represents a problem in which each of the six processing units interconnected in a flowsheet has three operating regions, each region with different mass balance coefficient in terms of the main product flowrate. The mass balance coefficients and the bounds for each of the flowrates are shown in Table 3.

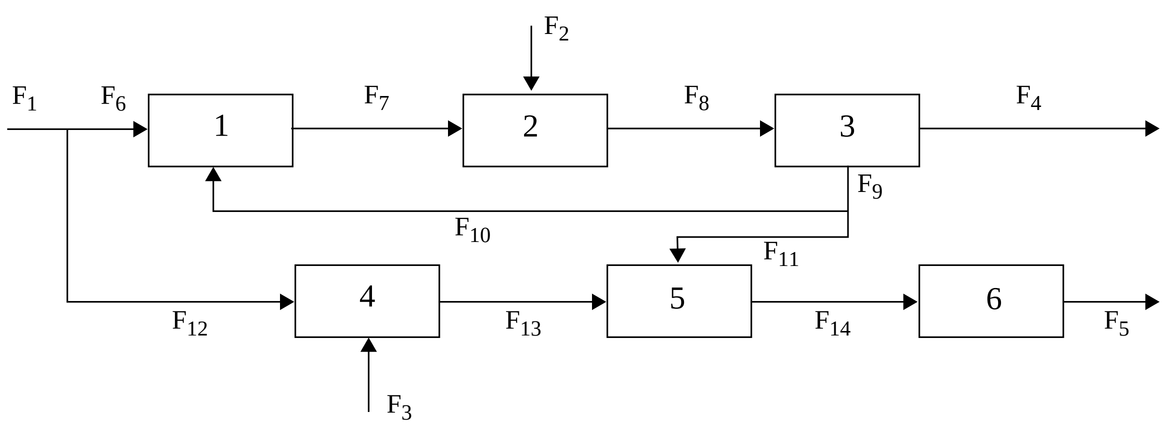

FIGURE 7 Processing Units for Example 6

Because of the three operating regions, the disjunctive linear mass balance for each of the units is represented for a disjunction containing 3 disjunctive terms. For instance, for the case of unit operation 1, we have:

$$\begin{bmatrix} F_6 = 1.1 \cdot F_7 \\ F_{10} = 0.05 \cdot F_7 \\ 0 \le F_7 \le 50 \end{bmatrix} \vee \begin{bmatrix} F_6 = 1.15 \cdot F_7 \\ F_{10} = 0.1 \cdot F_7 \\ 50 \le F_7 \le 80 \end{bmatrix} \vee \begin{bmatrix} F_6 = 1.2 \cdot F_7 \\ F_6 = 0.2 \cdot F_7 \\ 80 \le F_7 \le 150 \end{bmatrix}$$

Table 3: Material balance equations for units in Example 6

Unit	Main Product	Interval	Lower Bound	Upper Bound	Mass Balance Coefficient	
1	F_7	1	0	50	F_6: 1.10	F_{10}: 0.05
		2	50	80	1.15	0.10
		3	80	150	1.20	0.20
2	F_8	1	0	50	F_2: 0.50	F_7: 0.80
		2	50	100	0.47	0.75
		3	100	150	0.45	0.70
3	F_4	1	0	50	F_8: 1.70	F_9: 0.67
		2	50	110	1.80	0.70
		3	110	180	1.87	0.75
4	F_{13}	1	0	50	F_3: 1.18	F_{12}: 0.23
		2	50	90	1.15	0.25
		3	90	140	1.10	0.30
5	F_{14}	1	0	40	F_{11}: 0.37	F_{13}: 1.20
		2	40	80	0.35	1.25
		3	80	130	0.30	1.30
6	F_5	1	0	20	F_{14}: 1.15	
		2	20	45	1.10	
		3	45	75	1.02	

As a consequence of having three disjunctive terms, the formulation once again becomes complicated. Five out of the six units (those containing two equations in each term) can be represented by similar sets of disjunctive equations. For the case of unit 6 (which has only one equation in each disjunctive term), the disjunctive statement and the complementarity equations are similar from those obtained for the example of the simple flash calculation:

$$\begin{bmatrix} F_{14} = 1.15 \cdot F_5 \\ 0 \le F_5 \le 20 \end{bmatrix} \vee \begin{bmatrix} F_{14} = 1.10 \cdot F_5 \\ 20 \le F_5 \le 45 \end{bmatrix} \vee \begin{bmatrix} F_{14} = 1.02 \cdot F_5 \\ 45 \le F_5 \le 75 \end{bmatrix}$$

Even though the original problem is linear, the introduction of the complementarity equations leaves us with a nonlinear system of equations. The starting point used in this work and the converged values of the flowrates are shown in Table 4.

Table 4: Starting point and converged flowrates for Example 6.

Stream	Starting Point (lbmole/hr)	Converged Value (lbmole/hr)
F_1	47.50	47.5000
F_2	21.25	19.8549
F_3	69.00	57.7545
F_4	25.00	23.3587
F_5	50.00	36.5246
F_6	37.50	34.9447
F_7	34.00	31.7679
F_8	52.50	39.7099
F_9	16.75	15.6504
F_{10}	1.700	1.5884
F_{11}	16.80	14.0620
F_{12}	15.00	12.5553
F_{13}	60.00	50.2213
F_{14}	48.00	40.1770

3.1 ANALYSIS OF THE RESULTS

The number of iterations that we used to obtained the solution of each of these examples is shown in Table 5. Some observations are:

- The fixed parameters and constants for Examples 1 through 3 are the same as those giving by Zaher (1995).
- The number of iteration for the fluid transition problem corresponds to a diameter of 5 cm. For the example of the heat exchanger the number of iterations reported is for an area equal to 379.12 ft^2 and flowrate of cooling water equal to 1104.31 lbmole/hr. There is no special reason for the selection of those values . We just wanted to report a particular instance of the performance since the solution to these examples in the reference corresponds to optimization problems.
- For the simple flash calculation, the number of iterations reported is for the value of temperature of 200 K (liquid phase region). As before, there is no reason for using that value. The number of iterations was roughly of the same order for the rest of values of temperature.

Since the hardware and the technique that we are using to get the solution is different, we are comparing neither time nor number of iterations with other works. Still we consider it important to make remarks about some differences of the alternative approaches.

Table 5: Examples of algebraic systems of disjunctive equations found in the literature

Example	Reference	Number of Equations	Number of Disjunctions	Number of Complementarity Equations	Iterations
Fluid Transition	Zaher (1995)	7	1	1	8
Phase Equilibria	Zaher (1995)	18	3	3	10
Heat exchanger	Zaher (1995)	56	2	4	11
Pipeline network	Bullard and Biegler (1992)	250	38	76	24
Simple L-V flash	King (1980)	23	1	4	25
Linear mass balance	Grossmann and Turkay (1996)	81	6	34	25

In the example of the pipeline network, the result of the complementarity representation is one nonlinear system containing 250 equations, 76 of them containing 2 bilinear terms. In the same example, the number of boundaries in the boundary crossing algorithm (Zaher, 1991) would be 38 (that means 2^{38}=2.748779 x 10^{11} possible subregions) and the nonlinear system to be solved in every subregion would contain 98 equations. The combinatorial complications present in examples like this clearly represents a disadvantage for the boundary crossing algorithm. On the other hand, the reverse situation is also possible, and the boundary crossing may be clearly a better option than the complementarity formulation. For example, in a problem with only one disjunction, but 20 equations in each of the terms of the disjunction, we may not be able to solve a nonlinear system in which 20 of the equations contain 20 bilinear terms each. However, the number of subregions in the boundary crossing algorithm would be only 2, and the possibility of applying this algorithm efficiently would be much greater.

In the example of the linear mass balance, Turkay and Grossmann (1996) solve the problem by using a mixed-integer approach. The resulting MILP contains 18 binary variables, 66 continuous variables and 89 linear equations. In the complementarity formulation, the nonlinear system contains 81 equations, 47 are linear, but the remaining 34 contain multiplications among residuals. The size of the problem is very similar, the difference will be in either using a branch and bound search in the MILP or dealing with the complementarity equations in the solution of one square nonlinear system of equations.

4 CONCLUSIONS

We have proposed and tested a new representation of conditional models as complementarity problems. In order to obtain the complementarity formulation, we rely on the assumption that the sets of conditional equations are of the form $\underline{r}(\underline{x}):\boldsymbol{R}^n{}_+ \longrightarrow \boldsymbol{R}^n$ and, therefore, the disjunctive statements can be represented in terms of positive residual variables. We show that the formulation described in this paper does not introduce spurious solutions to the problem, and, under the assumption of nondegeneracy, it will not introduce numerical singularities to the Jacobian matrix. Also, for disjunctive statements having more than two terms, examples 5 and 6 show that sometimes it is possible to obtain a far less complex formulation than that obtained as a general formulation by taking advantage of the structure of the disjunctive representation. The number of iterations employed for all of the examples solved here makes the complementarity approach appear as an interesting alternative. We also mentioned some of the weaknesses and advantages of this approach.

5 ACKNOWLEDGMENTS

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6 REFERENCES

Billups, S. C.; Algorithms for Complementarity Problems and Generalized Equations. PhD thesis, University of Wisconsin-Madison, August 1995.

Bullard, L. G. and Biegler, L. T.; Iterative Linear Programming Strategies for Constrained Simulation. *Comput. Chem. Eng.*, 15(4):239–254, 1991.

Bullard, L. G. and Biegler, L. T.; Iterated Linear Programming Strategies for Nonsmooth Simulation: Continuous and Mixed-Integer Approach. *Comput. Chem. Eng.*, 16(10), 1992

Dirske, S. P. and Ferris, M. C.; MCPLIB: A Collection of Nonlinear Mixed Complementarity Problems. Optimization Methods and Software, 5, 1995.

Ferris, M. C. and Pang, J. S. ; Engineering and Economic Applications of Complementarity Problems. Technical report, University of Colorado, 1995.

Grossmann, I. E. and Turkay, M.; Solution of Algebraic Systems of Disjunctive Equations. *Comput. Chem. Eng.*, 20:S339–44, 1996. Suppl. Part A.

King, C. J.; Separation Processes, Chemical Engineering Series, 2nd. Edition, McGrawHill, 77-79, 1980.

Michelsen, M.L.; The Isothermal Flash Problem. Part I: Stability. *Fluid Phase Equilibria*, 9, 1-19, 1982.

More, J. J.; Global Methods for Nonlinear Complementarity Problems. Technical report, Argonne National Laboratory, Mathematics and Computer Science Division, April 1994.

Quesada, I. and Grossmann I. E.; A Global Optimization Algorithm for Linear Fractional and Bilinear Programs. *Journal of Global Optimization*, 6:39–76, 1995.

Viswanathan, J. and Grossmann, I. E.; A Combined Penalty Function and Outer Approximation Method for MINLP Optimization. *Comput. Chem. Eng.*, 14(7):769–782, 1990.

Westerberg, A. W. and Director, S. W.; A Modified Least Square Algorithm for Solving Sparse n x n Sets of Nonlinear Equations. Technical report, Carnegie Mellon University, Engineering Design Research Center, EDRC-06-5-79, January 1979.

Zaher, J. J.; Conditional Modeling. PhD thesis, Department of Chemical Engineering Carnegie Mellon University, Pittsburgh, Pennsylvania, May 1995.

Zaher, J. J.; Conditional Modeling in an Equation-Based Modeling Environment. The Annual AIChE National Meeting, 1991. paper 138c.

Zaher, J. J.; Conditional Programming. The Annual AIChE National Meeting, March 1993.

7 APPENDIX A

Complementarity Equations for the Examples presented in Section 3

Example 1 Fluid Transition (Zaher,1995).

A single complementarity equation is required. The definition of the positive residuals and the complementarity equation is given by:

$$1 - M_f = p_1^1$$

$$p_f - p_d = p_1^2$$

$$\begin{bmatrix} p_1^1 = 0 \\ p_1^2 \geq 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_1^1 \geq 0 \end{bmatrix} \quad \Longrightarrow \quad \begin{matrix} p_1^1 \cdot p_1^2 = 0 \\ p_1^1, p_1^2 \geq 0 \end{matrix}$$

Since the problem contains only one condition in each disjunctive term, our complementarity representation reduces to the standard complementarity formulation.

Example 2 Phase Equilibria (Zaher,1995).

The representation of the existence-non existence of each phase is given by the following set of equations.

$$\phi^A = p_1^1$$

$$1 - \sum_{i \in C} y_i^A = p_1^2$$

$$\begin{bmatrix} p_1^1 = 0 \\ p_1^2 \geq 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_1^1 \geq 0 \end{bmatrix} \quad \Longrightarrow \quad \begin{matrix} p_1^1 \cdot p_1^2 = 0 \\ p_1^1, p_1^2 \geq 0 \end{matrix}$$

The complementarity equation is entirely the same as in Example 1.

Example 3 Heat Exchanger (Zaher,1995).

$$\phi^0 = p_{11}^1 \qquad 1 - \sum_{i \in C} x_i^{\ 0} = p_{11}^2$$

$$\eta^1 = p_{21}^1 \qquad 1 - \sum_{i \in C} x_i^{\ 1} = p_{21}^2$$

$$\begin{bmatrix} p_{11}^1 = 0 \\ p_{21}^1 = 0 \end{bmatrix} \vee \begin{bmatrix} p_{11}^2 = 0 \\ p_{21}^2 = 0 \end{bmatrix} \Longrightarrow \begin{matrix} p_{11}^1 \cdot p_{11}^2 + p_{21}^1 \cdot p_{21}^2 = 0 \\ p_{11}^1 \cdot p_{21}^2 + p_{21}^1 \cdot p_{11}^2 = 0 \end{matrix}$$

$$\phi^1 = p_{12}^1 \qquad 1 - \sum_{i \in C} x_i^{\ 2} = p_{12}^2$$

$$\eta^2 - 0.5 = p_{22}^1 \qquad 0.5 - \eta^1 = p_{22}^2$$

$$\begin{bmatrix} p_{12}^1 = 0 \\ p_{22}^1 = 0 \end{bmatrix} \vee \begin{bmatrix} p_{12}^2 = 0 \\ p_{22}^2 = 0 \end{bmatrix} \Longrightarrow \begin{matrix} p_{12}^1 \cdot p_{12}^2 + p_{22}^1 \cdot p_{22}^2 = 0 \\ p_{12}^1 \cdot p_{22}^2 + p_{22}^1 \cdot p_{12}^2 = 0 \end{matrix}$$

$$p_{jk}^i \geq 0 \qquad \forall i \in [1\ldots2],\ j \in [1\ldots2],\ k \in [1\ldots2]$$

Example 4 Pipeline Network (Bullard and Biegler, 1992).

1) Arcs with no valve

$$H_{ij} + K \cdot Q_{ij}^{\ 2} = p_1^1$$

$$K \cdot Q_{ij}^{\ 2} - H_{ij} = p_1^2$$

$$Q_{ij} = p_2^1 - p_2^2$$

$$\begin{bmatrix} p_1^1 = 0 \\ p_2^1 = 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_2^2 = 0 \end{bmatrix} \Longrightarrow \begin{matrix} p_1^1 \cdot p_1^2 + p_2^1 \cdot p_2^2 = 0 \\ p_1^1 \cdot p_2^2 + p_2^1 \cdot p_1^2 = 0 \end{matrix}$$

$$p_j^i \geq 0 \qquad \forall i \in [1\ldots2],\quad j \in [1\ldots2]$$

and

2)Arcs with check valve

$$K \cdot Q^2{}_{ij} = p_1^1$$

$$K \cdot Q^2{}_{ij} - H_{ij} = p_1^2$$

$$H_{ij} = p_2^1 - p_2^2$$

$$\begin{bmatrix} p_1^1 = 0 \\ p_2^1 = 0 \end{bmatrix} \vee \begin{bmatrix} p_1^2 = 0 \\ p_2^2 = 0 \end{bmatrix} \quad \Longrightarrow \quad \begin{matrix} p_1^1 \cdot p_1^2 + p_2^1 \cdot p_2^2 = 0 \\ p_1^1 \cdot p_2^2 + p_2^1 \cdot p_1^2 = 0 \end{matrix}$$

$$p_j^i \geq 0 \qquad \forall i \in [1 \ldots 2]\ , \quad j \in [1 \ldots 2]$$

Example 5 Simple L-V Flash Calculation (King, 1980).

In this example, some of the residual variables p appear in more than one disjunctive term and a representation including an index i for each disjunctive term could be confusing. For that reason, we use the variables p indexed in successive order as follows:

$$V/F = p_1 \qquad V/F = R + p_2 - p_3 \qquad V/F = 1 - p_4$$

$$R = p_5 - p_6 \qquad R = 1 + p_7 - p_8$$

The disjunctive representation in terms of the residuals is:

$$\begin{bmatrix} p_1 = 0 \\ p_5 = 0 \\ p_3 = 0 \\ p_7 = 0 \end{bmatrix} \vee \begin{bmatrix} p_2 = 0 \\ p_6 = 0 \\ p_3 = 0 \\ p_7 = 0 \end{bmatrix} \vee \begin{bmatrix} p_2 = 0 \\ p_6 = 0 \\ p_4 = 0 \\ p_8 = 0 \end{bmatrix}$$

$$p_j \geq 0 \qquad \forall j \in [1 \ldots 8]$$

Note that several conditions appear in two different disjunctive terms. We could generate the complementarity equations as we described in section 2. The formulation obtained would still be consistent. However, we are concerned with the complications in the convergence of this kind of examples because the assumption of nondegeneracy does not hold and, therefore, numerical singularities could arise during the solution of the nonlinear system of equations.

Searching for a simplification which could help us to solve the problem, we took advantage of a very specific structure of the disjunctive representation given above. The following structure can be identified:

$$\begin{bmatrix} A \\ B \end{bmatrix} \vee \begin{bmatrix} C \\ B \end{bmatrix} \vee \begin{bmatrix} C \\ D \end{bmatrix} \qquad \Longrightarrow \qquad (A \wedge B) \vee (C \wedge B) \vee (C \wedge D)$$

and converting from Disjunctive Normal Form to Conjunctive Normal Form:

$$(A \wedge B) \vee (C \wedge B) \vee (C \wedge D) \qquad \Longrightarrow \qquad (A \vee C) \wedge (B \vee C) \wedge (B \vee D)$$

This derivation tells us that, in order to represent the three-term disjunctive term, we can use the union of two-term disjunctions:

$$\left\{ \begin{bmatrix} p_1 = 0 \\ p_5 = 0 \end{bmatrix} \vee \begin{bmatrix} p_2 = 0 \\ p_6 = 0 \end{bmatrix} \right\} \wedge \left\{ \begin{bmatrix} p_3 = 0 \\ p_7 = 0 \end{bmatrix} \vee \begin{bmatrix} p_2 = 0 \\ p_6 = 0 \end{bmatrix} \right\} \wedge \left\{ \begin{bmatrix} p_3 = 0 \\ p_7 = 0 \end{bmatrix} \vee \begin{bmatrix} p_4 = 0 \\ p_8 = 0 \end{bmatrix} \right\}$$

$$\left\{ \begin{array}{l} p_1 \cdot p_2 + p_5 \cdot p_6 = 0 \\ p_1 \cdot p_6 + p_5 \cdot p_2 = 0 \end{array} \right\} \wedge \left\{ \begin{array}{l} p_3 \cdot p_2 + p_7 \cdot p_6 = 0 \\ p_3 \cdot p_6 + p_7 \cdot p_2 = 0 \end{array} \right\} \wedge \left\{ \begin{array}{l} p_3 \cdot p_4 + p_7 \cdot p_8 = 0 \\ p_3 \cdot p_8 + p_7 \cdot p_4 = 0 \end{array} \right\}$$

If we do that for this example, the number of terms in our complementarity representation decreases significantly: strictly, a disjunction with three terms and four conditions in each term requires 4^3= 64 trilinear terms for its representation. On the other hand, the previous derivation tells us that 12 bilinear terms are enough for the representation of this particular problem.

We still need to find out how to distribute the 12 bilinear terms through the 4 complementarity equations required to obtain a square system of equations. Such a distribution is not unique, and we can use any set of complementarity equations which does not introduce numerical singularities (any set in which it can be proved that there is a possible pivot for each complementarity equation in the Jacobian matrix) to the system. The distribution can be as simple as the following:

$$p_1 \cdot p_2 + p_5 \cdot p_6 = 0$$

$$p_1 \cdot p_6 + p_5 \cdot p_2 = 0$$

$$p_3 \cdot p_2 + p_7 \cdot p_6 + p_3 \cdot p_4 + p_7 \cdot p_8 = 0$$

$$p_3 \cdot p_6 + p_7 \cdot p_2 + p_3 \cdot p_8 + p_7 \cdot p_4 = 0$$

$$p_j \geq 0 \qquad \forall j \in [1 \ldots 8]$$

in which the terms of two disjunctions are joined to generate two of the equations, or a more thoughtful one like:

$$p_1 \cdot p_2 + p_3 \cdot p_6 + p_7 \cdot p_8 = 0$$

$$p_1 \cdot p_6 + p_3 \cdot p_2 + p_7 \cdot p_4 = 0$$

$$p_5 \cdot p_2 + p_7 \cdot p_6 + p_3 \cdot p_4 = 0$$

$$p_5 \cdot p_6 + p_7 \cdot p_2 + p_3 \cdot p_8 = 0$$

$$p_j \geq 0 \qquad \forall j \in [1 \ldots 8]$$

in which the complementarity pairs are arranged to avoid repeated indices in the complementarity equations. When incorporated with the rest of the system, both sets of complementarity equations provide the correct solution to the problem. The number of iterations that we reported in this paper corresponds to the straightforward formulation given first.

Example 6 Linear Mass Balance (Grossmann and Turkay, 1996).

Once again, this example has disjunctions with 3 disjunctive terms. We only show the complementarity equations for unit operation 1. The equations for unit operation 2 to 5 are very similar to the equations generated for this one. Unit operation 6 has a representation similar to the disjunction of the Example 5. The simplification process for this example is the same as that given in Example 5. Definition of the residual variables:

$$F_6 = 1.1 \cdot F_7 + p_1 \qquad F_6 = 1.5 \cdot F_7 + p_2 - p_3 \qquad F_6 = 1.2 \cdot F_7 - p_4$$

$$F_{10} = 0.05 \cdot F_7 + p_5 \qquad F_{10} = 0.1 \cdot F_7 + p_6 - p_7 \qquad F_{10} = 0.2 \cdot F_7 - p_8$$

$$F_7 = 50 + p_9 - p_{10} \qquad F_7 = 80 + p_{11} - p_{12}$$

Disjunctive statement in terms of the residual variables:

$$\begin{bmatrix} p_1 = 0 \\ p_5 = 0 \\ p_9 = 0 \\ p_2 = 0 \\ p_6 = 0 \\ p_{11} = 0 \end{bmatrix} \vee \begin{bmatrix} p_3 = 0 \\ p_7 = 0 \\ p_{10} = 0 \\ p_2 = 0 \\ p_6 = 0 \\ p_{11} = 0 \end{bmatrix} \vee \begin{bmatrix} p_3 = 0 \\ p_7 = 0 \\ p_{10} = 0 \\ p_4 = 0 \\ p_8 = 0 \\ p_{12} = 0 \end{bmatrix}$$

After converting to Conjunctive Normal Form:

$$\left\{ \begin{bmatrix} p_1 = 0 \\ p_5 = 0 \\ p_9 = 0 \end{bmatrix} \vee \begin{bmatrix} p_3 = 0 \\ p_7 = 0 \\ p_{10} = 0 \end{bmatrix} \right\} \wedge \left\{ \begin{bmatrix} p_2 = 0 \\ p_6 = 0 \\ p_{11} = 0 \end{bmatrix} \vee \begin{bmatrix} p_3 = 0 \\ p_7 = 0 \\ p_{10} = 0 \end{bmatrix} \right\} \wedge \left\{ \begin{bmatrix} p_2 = 0 \\ p_6 = 0 \\ p_{11} = 0 \end{bmatrix} \vee \begin{bmatrix} p_4 = 0 \\ p_8 = 0 \\ p_{12} = 0 \end{bmatrix} \right\}$$

One possible set of Complementarity equations:

$$p_1 \cdot p_3 + p_2 \cdot p_4 + p_9 \cdot p_7 + p_6 \cdot p_{10} + p_{11} \cdot p_{12} = 0$$

$$p_1 \cdot p_7 + p_2 \cdot p_8 + p_9 \cdot p_{10} + p_6 \cdot p_3 + p_{11} \cdot p_4 = 0$$

$$p_1 \cdot p_{10} + p_2 \cdot p_{12} + p_9 \cdot p_3 + p_6 \cdot p_7 + p_{11} \cdot p_8 = 0$$

$$p_5 \cdot p_3 + p_6 \cdot p_4 + p_{11} \cdot p_{10} + p_2 \cdot p_7 = 0$$

$$p_5 \cdot p_7 + p_6 \cdot p_8 + p_{11} \cdot p_3 + p_2 \cdot p_{10} = 0$$

$$p_5 \cdot p_{10} + p_6 \cdot p_{12} + p_{11} \cdot p_7 + p_2 \cdot p_3 = 0$$

$$p_j \geq 0 \qquad \forall j \in [1 \ldots 12]$$

The number of iterations reported in this paper corresponds to the solution of the system of equations including this set of complementarity equations, but some other alternative sets were also successfully used to obtain the solution to the problem