Structural analysis of Conditional Models

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Abstract: Structural analysis is applied to exploit sparsity in the solving of a system of equations (Duff et al. 1989). Zaher (1995) studied the issues involved in the structural analysis of conditional models and presented a methodology to ensure consistency in a conditional model, the complexity of such an analysis being combinatorial. In that work, Zaher considered only cases in which the number of variables and equations of all the alternatives in a conditional model are the same. In this chapter, an extension to Zaher’s consistency analysis is presented. This extension allows the consistency analysis to be applied to conditional models in which the number of variables and equations for each of the alternatives may not be the same. Also, we show how, by taking advantage of the structure of the problem, it is sometimes possible to reduce the effort required by such an analysis. In particular, the cases of the existence of repeated structures and common incidence pattern among alternatives are discussed.

Keywords: Structural Analysis, variable partitioning, conditional models.

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1 INTRODUCTION/MOTIVATION

Before attempting to solve a model, a structural analysis has to be performed to determine if the model formulation is well posed. Techniques are available which can be used to detect if any structural inconsistency exists among the equations of the model (Duff et al., 1989; Zaher, 1995). However, consistency is generally assumed and structural analysis is rarely discussed in the literature.

Still, in practice it is very difficult to create large models of equations without introducing structural inconsistencies. We believe that structural analysis is an indispensable tool in an equation-based modeling environment, and, as we show in section 3, conditional models make the need for this tool an even stronger requirement.

2 TERMINOLOGY IN STRUCTURAL ANALYSIS

We provide here a brief and general description of the terminology employed throughout this paper. Also, we use the system of equations given in Example 1 to illustrate each of the definitions.

Variables appearing in an equation are said to be incident in that equation and incident in the problem containing that equation. Assume that \( m \) is the number of equations in a model and \( n \) is the number of variables incident in those equations. For most engineering models, \( n > m \). In order to solve a problem, the problem has to be square; that is, the number of equations and the number of variables to be calculated in the problem has to be the same. Accordingly, in order to solve a problem containing \( n \) variables and \( m \) equations, it is necessary to provide the values of \( n-m \) variables, so that we can calculate the rest. Thus, the difference between the number of variables and the number of equations gives us the number of degrees of freedom, \( DOF=n-m \), of the problem. The \( m \) variables to be calculated in the problem are called dependent variables, while the \( n-m \) variables whose values are provided by the modeler are called independent or decision variables. Because of structural considerations (as we explain below), not every variable can be designated an independent variable. The set of variables whose values can be provided by the modeler (that is, the set of candidates to become an independent variable) is called the eligible set.
EXAMPLE 1 A System of Equations to Illustrate the Terminology in Structural Analysis.

\[
\begin{align*}
   x_1 = 1 & \quad f_1 = x_1 - 1 = 0 \\
   x_2 + x_4 = 5 & \quad f_2 = x_2 + x_4 - 5 = 0 \\
   x_3 - x_4 + x_2 = 3 & \quad f_3 = x_3 - x_4 + x_2 - 3 = 0 
\end{align*}
\]

For the system of equations in Example 1:

Set of incident variables in first equation = \{x_1\}

Set of incident variables in the problem = I = \{x_1, x_2, x_3, x_4\}

Number of variables in the problem = n = 4

Number of equations in the problem = m = 3

Number of degrees of freedom = DOF = 4 - 3 = 1

The equations of a model are expected to have different sets of variables incident in them. Furthermore, they are expected to involve only a few of the variables in the problem. This observation supports the idea that models are sparse. An effective representation of a sparsity pattern of a system of equations is given by an incidence matrix. The rows of an incidence matrix correspond to the equations of the problem. Similarly, the columns of an incidence matrix correspond the variables incident in the equations. An element in row i and column j of an incidence matrix is nonzero if and only if the variable of column j is incident in the equation of row i. The incidence matrix of the system of equations given by Example 1 is shown in Figure 1.

FIGURE 1 Incidence matrix of Example 1.

<table>
<thead>
<tr>
<th>( f_1 )</th>
<th>( f_2 )</th>
<th>( f_3 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( x_1 )</td>
<td>\bullet\</td>
<td>\bullet\</td>
</tr>
<tr>
<td>( x_2 )</td>
<td>\bullet\</td>
<td>\bullet\</td>
</tr>
<tr>
<td>( x_3 )</td>
<td>\bullet\</td>
<td>\bullet\</td>
</tr>
<tr>
<td>( x_4 )</td>
<td>\bullet\</td>
<td>\bullet\</td>
</tr>
</tbody>
</table>
Structural inconsistencies are detected by using an incidence matrix to perform an output assignment. An output assignment is the process of assigning each equation to one of its incident variables. The structural rank is the largest number of equations which can be assigned such that no two equations are assigned to the same variable. If rank = m, the system of equations is structurally consistent. If, on the other hand, rank < m, the equations are guaranteed to be singular. An output assignment for the system given in Example 1 is shown in Figure 2.

**FIGURE 2** An output assignment for the system defined in Example 1.

<table>
<thead>
<tr>
<th></th>
<th>x₁</th>
<th>x₂</th>
<th>x₃</th>
<th>x₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>f₁</td>
<td></td>
<td>☐</td>
<td></td>
<td></td>
</tr>
<tr>
<td>f₂</td>
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<tr>
<td>f₃</td>
<td>☐</td>
<td>☐</td>
<td>☐</td>
<td>☐</td>
</tr>
</tbody>
</table>

Besides the detection of structural inconsistencies, the output assignment also provides a solid basis for finding a consistent partitioning of the variables. After a structurally consistent output assignment is achieved, the variables which are assigned make up a consistent set of dependent variables, while the variables left to be assigned make up a set of independent or decision variables. However, the partitioning of the variables is not unique and a generalized criterion to select the best choice does not exist. Hence, it is important to generate and make available all of the choices to the modeler. All the candidates to become independent variables can be found from an initial output assignment by following Steward paths (Westerberg et al., 1979). A Steward path starts from an unassigned independent variable and then moves horizontally to an assigned variable, then vertically to an unassigned variable, then horizontally to an assigned variable, etc., until the path terminates, always on an assigned variable. The variables encountered along each path are marked as being eligible. Thus, all the variables gathered while transversing all of the Steward paths constitute the eligible set of variables in the problem being analyzed. A Steward path is illustrated in Figure 3. The combined use of an output assignment and Steward paths to obtain the eligible set is called an eligibility analysis.
The eligible set of variables for the problem of Example 1 is:

\[ E = \{x_2, x_3, x_4\} \]

For the system of equations given in Example 1, selecting one of the variables in the eligible set \( E \) as being an independent variable results in a square structurally consistent system of equations.

### 2.1 Notation

The following notation is used in the remainder of this paper. For an alternative set of equations \( i \) where \( i \in \{1 \ldots s\} \), and \( s \) is the number of alternatives in a conditional model:

- \( E_i \): Eligible set - Set of variables eligible to be chosen as independent variables in the alternative \( i \).
- \( I_i \): Incidence set - Set of variables incidents in the equations constituting the alternative \( i \).
- \( M \): Maximal set - Union of the incidence sets of all of the alternatives.
- \( DOF_i \): Number of degrees of freedom left to be assigned.
- \( e \): Intersection of the eligible sets of all the alternatives.

While assigning degrees of freedom in a structural analysis, every time that a variable is chosen to be an independent variable, the elements change in the eligible set for the selection of the remaining degrees of freedom. The number of elements in the new eligible set is at least one less than the previous set. Moreover, the new eligible set is always a subset of the eligible set previous to the selection of the independent variable. For that reason, we use the index \( k \) to indicate a \( k-th \) step in the selection of the independent variables while performing structural analysis. Note that
the sets $I_i$ and $M$ are independent of this index $k$, while the sets $E_i$ and their intersection $e$ change at each step $k$.

$k$ \( k-th \) step in the assignment of the degrees of freedom.

2.1.1 Set Operators

- **Union**  \( A \cup B \) is all elements either in $A$, $B$, or both.

- **Intersection**  \( A \cap B \) is all elements in both $A$ and $B$.

- **Minus**  \( A \setminus B \) is all elements from $A$ not in $B$.

3  **STRUCTURAL CONSISTENCY**

Duff *et al*. (1989) and Zaher (1995) describe algorithms for the systematic structural consistency analysis in conventional models. They give a step by step procedure to:

- Generate an incidence matrix.
- Perform an output assignment in order to test structural consistency.
- Collect all the eligible variables by following all the Stewards path in a problem.

The interested reader may refer to those works for a detailed description of the procedures. Our attention in the rest of this paper is focused in the structural consistency of conditional models.

3.1  **CONDITIONAL MODELS**

In conditional models, the sparsity pattern is expected to change from one alternative set of equations to another. This implies that a consistent set of independent variables for one alternative set of equations may not be valid for another one.

Zaher (1993, 1995) also addressed the structural analysis of conditional models. A necessary condition for structural consistency in conditional models is that each of the alternative sets of equations must be structurally consistent. Hence, consistency of a conditional model is assessed by finding at least one consistent partitioning of the variables (independent-dependent) such that output assignment of all of the equations in each alternative can be performed. This requirement makes the problem combinatorial, since we have to perform the analysis for all of the alternative
sets of equations which can be generated from a conditional model expressed disjunctively. The following is an abbreviated description of an algorithm for finding a set of independent variables consistent with all the alternative sets of a conditional model. For a detailed description, see Zaher (1995). It is assumed that there is a nonzero number of degrees of freedom in the problem:

1. Each of the alternative sets of equations is first arbitrarily output assigned.
2. For each output assignment, the set of variables eligible to become independent \((E^k_i)\) is generated. In general, the eligible sets generated for each of the alternatives are different.
3. Since, it is necessary (but not sufficient) that a variable which is eligible in the context of the overall problem must be eligible for each alternative, we next find the intersection of the eligible sets generated in step 2:

\[
e^k = E^k_1 \cap E^k_2 \cap \ldots \cap E^k_s = \bigcap_j^{s} E^k_j
\]  

(1)

where \(s\) the number of alternatives in the conditional model.
4. We tentatively select a variable from the intersection set generated in step 3 to be an independent variable. After this step, the number of independent variables left is reduced by one, and the process is repeated from step 1 using the remaining dependent variables.
5. Consistency is achieved only if a sequence is found which allows an eligible variable to be selected for each degree of freedom. Therefore, we backtrack anytime we fail to complete such a sequence.

### 3.1.1 Limitations of Zaher’s Consistency Analysis

Consider a conditional model in which ‘s’ alternative sets of equations can be generated. In his work, Zaher only addressed the case in which the variables incident in each of the alternatives is the same,

\[
I_1 = I_2 = \ldots = I_s = I
\]

Given that condition, the variables common to all of the eligible sets of each alternative set of
equations \( (e^k) \) can be regarded as eligible to become independent in the context of the overall conditional model.

In a general situation, however, the number of equations in each alternative of a conditional model may change and so may the incidence set of variables.

4 \hspace{1cm} \textbf{EXTENSION OF THE CONSISTENCY ANALYSIS FOR CONDITIONAL MODELS}

For the case developed by Zaher in which the incident variables of all the alternatives are the same, the result of applying equation (1) is the elimination of all those variables which are eligible to be chosen as independent variables in some alternatives but non eligible to be chosen as independent variables in some other alternatives. That is readily accomplished by using the intersection of the individual eligible sets since all the variables are incident in all the alternatives.

For the general case, however, since we expect

\[ I_1 \neq I_2 \neq I_3 \ldots \neq I_s \]

we cannot use the intersection of the eligible set of each alternative to generate the eligible set for the overall conditional model. If we would do that, we would immediately remove variables which are not incident in some of the alternatives, since they would not be eligible for an alternative in which they are not incident.

A detailed derivation of an equivalent to (1) when the alternatives of a conditional model have different incident variables is presented in Appendix A. In Appendix A, we show that, in general, for any alternative \( i \in \{ 1 \ldots s \} \), the set of “truly” eligible variables (ineligible variables are eliminated) for each alternative in the context of the overall conditional problem is given by:

\[
E_{i'}^k = E_i^k \{ E_i^k \cap \left[ \bigcup_{j, j \neq i}^s (I_j \setminus E_j^k) \right]\}
\]

and that the union of these individual sets gives the set of eligible variables from which we can safely select the independent variables of a conditional model:
Hence, by using (3) instead of (1), we can apply the structural consistency algorithm described in 3.1 to a general conditional model having alternatives with different incident variables.

Furthermore, in Appendix A we also show that we do not have to perform the analysis for the general case as defined in (3). A simpler analysis can be used instead. We demonstrate that, if we augmented the eligible set of each alternative $E^{k}_{i}$ with the non incident variables of that alternative:

\[ E^{k'''}_{i} = E^{k}_{i} \cup (M \setminus I_{i}) \]  

(4)

and find the intersection of the augmented sets $E^{k'''}_{i}$,

\[ e^{k'''} = \bigcap_{i} E^{k'''}_{i} = \bigcap_{i} [E^{k}_{i} \cup (M \setminus I_{i})] \]  

(5)

then the resulting set $e^{k'''}$ is equivalent to the set $e^{k'}$ given by (3). Recall that $M$ is the maximal set of variables,

\[ M = I_{1} \cup I_{2} \cup \ldots I_{s} = \bigcup_{j} I_{j} \]  

(6)

so that $(M \setminus I_{i})$ represents the set of non incidences in alternative $i$.

Therefore, the use of (5) instead of (1) also allows us to apply the structural consistency algorithm described in 3.1 to a general conditional model having alternatives with different incident variables. As a final result in Appendix A, we also demonstrate that both (5) and (3) reduce to (1) when the alternatives of a conditional model have the same incident variables.
4.1 THE MAIN RESULT

The main result of the analysis presented in this section is that the algorithm described in section 3.1, derived for a conditional model having the same incident variables in all its alternative set of equations, can still be applied for a general case in which different alternatives of a conditional model have different incident variables. In order to accomplish that, the step 3 of the algorithm for testing structural consistency given in 3.1 has to be modified by using (5) instead of (1).

4.2 AN IMPLEMENTATION

Our extension to the consistency analysis described in 3.1 has been incorporated as a tool within the ASCEND modeling environment to help a user to set up structurally consistent conditional models. Essentially, this implementation uses the information provided by the conditional statements described in Rico-Ramirez et al. (1998) in order to generate the alternative configurations of a conditional model. Then, for each of the alternatives, we apply the eligibility analysis techniques already available for conventional models.

4.3 AN ILLUSTRATIVE EXAMPLE

The formulation derived in this section is illustrated with Example 2. In this case, a disjunctive system of equations contains two disjunctions, which results in 4 different alternative set of equations. The 4 set of equations derives from Example 2 are shown in Figure 4.

For the purpose of illustration, assume that the variables $x_2$, $x_4$, and $x_7$ have already been selected as independent variables. Hence, the set of independent variables, $\mathcal{Q}$, prior to the analysis is:

$$\mathcal{Q} = \{x_2, x_4, x_7\}$$
EXAMPLE 2 A simple disjunctive set of equations.

\[
\begin{align*}
x_{18} &= 1 \\
x_1 &= 0.8 \cdot x_2 \\
x_3 &= 10 - x_4 \\
x_5 &= x_1 + x_3 \\
x_6 &= x_5 - x_1 \\
x_8 &= x_7 + x_6 \\
x_{12} &= 3 \cdot x_{21} \cdot x_3 \\
x_{14} &= x_7 + x_8 \\
x_{16} &= x_{24} + x_{11} \\
x_{15} &= x_{16} + x_{23} \\
x_{23} &= x_4
\end{align*}
\]

\[
\begin{align*}
x_7 &= 0.9 \cdot x_8 \\
x_9 &= x_8 + x_{10} + x_3 \\
x_{10} &= 40 - x_9 \\
x_{13} &= x_{21} \\
x_{17} &= x_7 \\
x_{19} &= x_{20} \\
x_{20} &= x_{22}
\end{align*}
\]

FIGURE 4 4 Alternatives in the Example 2.
Table 1 shows an analysis of the degrees of freedom left to be assigned for each of the alternatives. Note that the number of equations, the number of incident variables, and the number of degrees of freedom left to be assigned are different for each alternative.

<table>
<thead>
<tr>
<th>Alternative</th>
<th>Number of equations</th>
<th>Number of incidences</th>
<th>Number of DOF</th>
<th>DOF left to be assigned</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>11</td>
<td>17</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>9</td>
<td>13</td>
<td>4</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>12</td>
<td>18</td>
<td>6</td>
<td>3</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
<td>15</td>
<td>5</td>
<td>2</td>
</tr>
</tbody>
</table>

The eligible set for each of the alternatives, obtained from the eligibility analysis we described, is shown in Table 2.

<table>
<thead>
<tr>
<th>Alternative</th>
<th>Incidences, $I_i$</th>
<th>Eligible set, $E_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$x_1, ..., x_8, x_{11}, x_{12}, x_{14}, ..., x_{18}, x_{21}, x_{23}, x_{24}$</td>
<td>$x_{11}, x_{12}, x_{15}, x_{16}, x_{21}, x_{24}$</td>
</tr>
<tr>
<td>2</td>
<td>$x_1, ..., x_8, x_{17}, ..., x_{20}, x_{22}$</td>
<td>$x_{19}, x_{20}, x_{22}$</td>
</tr>
<tr>
<td>3</td>
<td>$x_1, ..., x_4, x_7, ..., x_{16}, x_{18}, x_{21}, x_{23}, x_{24}$</td>
<td>$x_{11}, x_{12}, x_{13}, x_{15}, x_{16}, x_{21}, x_{24}$</td>
</tr>
<tr>
<td>4</td>
<td>$x_1, ..., x_4, x_7, ..., x_{10}, x_{13}, x_{17}, ..., x_{22}$</td>
<td>$x_{13}, x_{19}, x_{20}, x_{21}, x_{22}$</td>
</tr>
</tbody>
</table>

If we would try to apply Zaher’s structural analysis in order to obtain a consistent set of independent variables for the overall problem, we would conclude structural inconsistency, since the intersection of the individual eligible sets is empty:

$$e^k = \bigcap_{j=1}^s E_j^k = \emptyset$$
Instead, we can apply either of the equations derived in this section to obtain:

from (3),

\[ e^{k'} = \bigcup_{i} E_{i}^{k'} = \{ x_{11}, x_{12}, x_{13}, x_{15}, x_{16}, x_{19}, x_{20}, x_{21}, x_{22}, x_{24} \} \]

or, from (5),

\[ M = \{ x_{1} \ldots x_{24} \} \]

\[ e^{k''} = \bigcap_{i} E_{i}^{k''} = \{ x_{11}, x_{12}, x_{13}, x_{15}, x_{16}, x_{19}, x_{20}, x_{21}, x_{22}, x_{24} \} \]

Note that the result is the same, \( e^{k'} = e^{k''} \). By applying the consistency algorithm in 3.1, we obtain the following set of consistent independent variables:

\[ \{ x_{11}, x_{15}, x_{19}, x_{21} \} \]

Hence, if we partition the variables in Example 2, so that the set of independent variables is given by,

\[ \mathcal{O} = \{ x_{2}, x_{4}, x_{7}, x_{11}, x_{15}, x_{19}, x_{21} \} \]

then all 4 alternatives generated from Example 2 are square and structurally consistent.

### 4.4 IS THE COMBINATORIAL CONSISTENCY ANALYSIS REALLY NECESSARY?

Given the combinatorial nature of conditional models, it may happen that, during the iterative solution of one of such models, only a few of the alternatives of it are considered before converging to the solution. For that reason, a question comes to mind. Why should we look for the structural consistency of all of the alternatives in a conditional model if it is true that many of those alternatives will never be encountered during an iterative solution technique?

First, we should recognize that it is also true that, in general, there is no way of knowing which alternatives will be visited during an iterative solution of a conditional model.
Simplifying the Consistency Analysis of Conditional Models

The analysis required for partitioning the variables in a conditional model was outlined in section 3.1. We see the most serious disadvantage of this analysis to be the combinatorial nature of the search consistency algorithm, which requires the analysis of all of the alternatives every time that a selection of an independent variable is made.

However, we have observed special features of some problems which can contribute to simplifying the analysis. Even though they represent very particular cases, if found alone or in any combination, we can take advantage of them in order to reduce the computational effort needed to perform the analysis.

5.1 Common Incidence Pattern

It happens sometimes that the equations of some alternatives in a conditional model are different only because of the difference in value of some parameters, such as cost factors, mass balance coefficients, power of a correlation, etc. That is, the incidence pattern of those alternatives is the same. In such a case, the combinatorial structural analysis can be greatly simplified. Consider the conditional model defined in Example 3. In that example, there are 6 disjunctions in the problem. Hence, the number of alternative set of equations is:

\[ Number \ of \ alternatives = 2^6 = 64 \]
EXAMPLE 3 Taking advantage of a common incidence pattern.

\[
\begin{align*}
    x_1 &= x_6 + x_{12} \\
    x_9 &= x_{10} + x_{11} \\
    x_6 &= 1.15 \cdot x_7 \\
    x_{10} &= 0.1 \cdot x_7 \\
    x_7 &\leq 8 \\
    x_6 &= 1.2 \cdot x_7 \\
    x_{10} &= 0.2 \cdot x_7 \\
    x_7 &\geq 8 \\
    x_2 &= 0.47 \cdot x_8 \\
    x_7 &= 0.75 \cdot x_8 \\
    x_8 &\leq 10 \\
    x_2 &= 0.45 \cdot x_8 \\
    x_7 &= 0.7 \cdot x_8 \\
    x_8 &\geq 10 \\
    x_8 &= 1.8 \cdot x_4 \\
    x_9 &= 0.7 \cdot x_2 \\
    x_4 &\leq 11 \\
    x_8 &= 1.87 \cdot x_4 \\
    x_9 &= x_1 \\
    x_4 &\geq 11 \\
    x_3 &= 1.15 \cdot x_{13} \\
    x_{12} &= 0.25 \cdot x_{13} \\
    x_{13} &\leq 9 \\
    x_3 &= 1.10 \cdot x_{13} \\
    x_{12} &= 0.3 \cdot x_{13} \\
    x_{13} &\geq 9 \\
    x_{11} &= 0.35 \cdot x_{14} \\
    x_{13} &= 1.25 \cdot x_{14} \\
    x_{14} &\leq 8 \\
    x_{11} &= 0.3 \cdot x_{14} \\
    x_{13} &= 1.3 \cdot x_{14} \\
    x_{14} &\geq 8 \\
    x_{14} &= 1.10 \cdot x_5 \\
    x_5 &\leq 4 \\
    x_{14} &= 1.02 \cdot x_5 \\
    x_5 &\geq 4
\end{align*}
\]

However, it is trivial to observe that, in all but one of the disjunctions, the incidence pattern is the same. As a consequence, for the purposes of structural analysis, only two different alternatives have to be considered.

\[
\text{Number of alternatives for structural analysis} = 2^1 = 2
\]

Hence, for instance, the structural analysis for the problem of Example 3, could be simplified to one of the system of equations shown in Figure 5.

5.1.1 An Implementation

In parallel with the implementation of our extension to the consistency analysis of a conditional model, we have also implemented a computer tool whose goal is identifying all those conditional structures with the same incidence pattern. This tool has been incorporated within the ASCEND
environment. It uses the information provided by the conditional statements described in Rico-Ramirez et al. (1998) (WHEN statement) in order to compare the incidence pattern of alternative configurations. This tool is applied as a step prior to the consistency analysis described in section 4. Hence, the consistency analysis considers only those alternatives whose incidence patterns are different, and, therefore, the combinatorial complexity of the analysis is reduced.

### 5.2 Repeated Structures

In chemical engineering design and simulation, systems containing repeated structures occur very often. Typical examples are a distillation column (n trays) and systems of equations arising in the discretization of an initial value problem. If we think of a problem in which a disjunction exists in each of the repeated structures, the combinatorial complexity of the consistency analysis would be unmanageable. However, intuition suggests that, in these kinds of problems, the degrees of freedom analysis should not be affected by the number of repeated structures and, therefore, the analysis could be simplified. Based on the work of Allen and Westerberg (1976), we show here that sometimes it is possible to take considerable advantage of the existence of repeated structures in a conditional model, reducing the effort required by the consistency analysis.

\[
\begin{align*}
x_1 &= x_6 + x_{12} \\
x_9 &= x_{10} + x_{11} \\
x_6 &= 1.15 \cdot x_7 \\
x_{10} &= 0.1 \cdot x_7 \\
x_2 &= 0.47 \cdot x_8 \\
x_7 &= 0.75 \cdot x_8 \\
x_8 &= 1.8 \cdot x_4 \\
x_9 &= 0.7 \cdot x_2 \\
x_3 &= 1.15 \cdot x_{13} \\
x_{12} &= 0.25 \cdot x_{13} \\
x_{11} &= 0.35 \cdot x_{14} \\
x_{13} &= 1.25 \cdot x_{14} \\
x_{14} &= 1.10 \cdot x_5
\end{align*}
\]
5.2.1 An Approach for Conventional Models

In their work, Allen and Westerberg used a representative incidence matrix to perform a systematic analysis of a conventional model containing repeated structures. They provide a criterion to decide whether or not, after a consistent output assignment has been found for the representative matrix, the result obtained for the representative matrix can be expanded to a system containing any number of the repeated structures. Consider the simple case illustrated in Figure 6. In this example, the output assignment of a system containing two equations has been performed, resulting in the selection of a structurally consistent set of 3 independent variables (marked as I in Figure 6). The problem consists in finding if we can expand this partitioning to a system containing \( n \) blocks of the same two equations. First, it is necessary to introduce the definition of the *modulo* of the expansion. Modulo is the number of positions that each new block added to the structure is going to move from the left-most entry (or right-most entry if the expansion is upward) of the previous block. In other words, modulo is the number of columns that each new block is going to be displaced with respect to the previous one. In the case of Figure 6, the modulo of the expansion is equal to 3.

Once the modulo of the expansion is known, Allen and Westerberg propose to enumerate the columns of the representative block successively from 0 to *modulo-1* until reaching the last column of the block. Then, the necessary condition for expanding the result to \( n \) blocks is that no two columns representing a dependent variable in the representative matrix can have the same column number. In Figure 6, this criterion is satisfied since the two columns representing the dependent variables has been enumerated as 1 and 0, and, therefore, the expansion can take place. Practically speaking, what this condition means is that we cannot allow, after an expansion to \( n \) blocks, the overlapping of any two columns chosen as dependent variables. If we allow that, we would have a variable assigned to more than one equation, a situation that violates the structural consistency requirement explained in section 2 (definition of the output assignment).
5.2.2 Equation-Based Modeling and the Modulo of Repeated Structures

In the context of an equation-based modeling, the set of overlapping variables and, therefore, the modulo of an array of repeated structures, are given by the connections among the repeated structures. In most of the existing equation-based environments currently available, there exist language constructs which allow the representation of connections defining the flow of information. So, for instance the IS operator of gPROMS (Barton, 1992) and the ARE_THESAME operator of ASCEND (Piela, 1989) serve this purpose.

5.2.3 Repeated Structures Containing Conditional Equations

As stated earlier, the combinatorial complexity of the consistency analysis of systems containing repeated structures with conditional equations would be practically unmanageable.

What we propose here is to perform the consistency analysis of this type of conditional model by using a representative structure of the problem. The difference with respect to the work presented by Allen and Westerberg is that, in our problem, the basic structure to be considered in the analysis contains conditional equations, and, therefore, a consistency analysis over all the possible
configurations of the representative structure has to be performed. In other words, we combine the consistency analysis developed for conditional models with the idea of analyzing only a representative block of an array of repeated structures. Example 4 and Example 5 illustrate the application of this approach.

5.2.4 Illustrative Examples

Example 4 is used to illustrate an extreme case, in which there may be sets of nested repeated structures containing conditional equations. We use indices $n$ and $m$ to indicate the number of repeated structures in each of the sets.

Example 4 Taking advantage of repeated structures.

\[
\begin{align*}
  x_1 + x_{2,1} &= 4 \\
  x_{2,1} - 2 \cdot x_1 &= 7 \\
  x_{2,1} - x_{3,1} + x_{4,1} &= 3 \\
  \left[ x_{6_{ij}} + x_{5_{ij}} + x_{6_{ij}} + x_{8_{ij}} = 9 \right] \\
  x_{6_{ij}} + x_{7_{ij}} - x_{3_{ij}} - x_{5_{ij}} &= 1 \\
  x_{6_{ij}} + x_{5_{ij}} - x_{6_{ij}} + x_{7_{ij}} &= 2 \\
  \forall j \in \{1 \ldots m\} \\
  x_{3_{j,1}}, x_{6_{j,1-1}} &\text{ATS} \\
  x_{4_{j,1}}, x_{5_{j,1-1}} &\text{ATS} \\
  x_{5_{j,1}}, x_{8_{j,1-1}} &\text{ATS} \\
  \forall j \in \{2 \ldots m\} \\
  x_{3_{j,1}}, x_{6_{j,1-1}} &\text{ATS} \\
  x_{4_{j,1}}, x_{5_{j,1-1}} &\text{ATS} \\
  x_{5_{j,1}}, x_{8_{j,1-1}} &\text{ATS} \\
  \forall i \in \{1 \ldots n\} \\
  x_{2_{i,1}}, x_{6_{i-1,m}} &\text{ATS} \\
  x_{3_{i,1}}, x_{7_{i-1,m}} &\text{ATS} \\
  x_{4_{i,1}}, x_{8_{i-1,m}} &\text{ATS} \\
  x_{6_{n,m}} - x_{7_{n,m}} - x_{8_{n,m}} &= 2 \\
  x_{6_{n,m}} - x_{7_{n,m}} &= 4 \\
\end{align*}
\]

For simplicity in the representation, the abbreviation ATS (ARE_THE_SAME, following the ASCEND modeling language representation) is used to express the connectivity among the variables incident in the repeated structures. The number of alternatives in problems of this nature grows...
very quickly with the number of repeated structures. So, for instance, if $m=5$ and $n=5$, the number of alternatives is:

$$\text{number of alternatives} = (2^5)^5 = 33554432$$

In order to structurally analyze this conditional model, we use a representative structure of the problem. For this case, this representative structure is given for a system in which $n=m=1$. The resulting system of equations is given in (7), where the subindexes $n=m=1$ have been omitted for simplicity.

$$\begin{align*}
x_1 + x_2 &= 4 \\
x_2 - 2 \cdot x_1 &= 7 \\
x_2 - x_3 + x_4 &= 3 \\
x_4 + x_5 + x_6 + x_8 &= 9 \\
x_6 + x_7 - x_3 - x_5 &= 1 \\
\end{align*}$$

The representative structure (7) contains 4 alternatives, each of them with one degree of freedom. By applying the structural consistency algorithm to the simplified problem, we obtain that the eligible set of the representative conditional model is:

$$\text{eligible set} = \{x_3, x_4, x_5, x_6, x_7, x_8\}$$

The task is to find a set of independent variables (only one variable in this example) which, for each alternative, allows us an output assignment satisfying Allen’s necessary conditions for expanding the result of a representative incidence matrix. For the representative conditional structure of Example 4, assigning $x_5$ as independent variable allows the output assignments presented in Figure 7 for each of the alternatives.
All 4 output assignments of Figure 7 satisfy Allen’s necessary conditions. Figure 8 illustrates the case of the nested blocks of alternative 1. The modulo of each block was determined by the connectivity among the repeated structures described in the formulation of Example 4.

We could show that, if we expand the result of the representative incidence matrix to any number of repeated structures and in any combination, the resulting systems of equations are still structurally consistent. Figure 9 shows an example of this expansion. Note that each variable $x_{5_{1,1}}$
is selected as independent variable (that is, it is not assigned).

**FIGURE 9** Expanding the result of a representative matrix. Expansion of alternative 1 with $n=m=2$.

The final example of this paper, Example 5, corresponds to a chromatographic separation performed in CCD (Craig Countercurrent Distribution) discussed by King (1980). This example is illustrated in Figure 10. At discrete intervals, transfers of the upper phase take place from one vessel to the next. Among these transfer steps, the upper phase then present in each vessel is equilibrated with the lower phase in that vessel. A small amount of feed mixture is initially present in the first vessel and then carried along from vessel to vessel in the distribution process. For a component $A$ being separated, the formulation is presented in Example 5.

**FIGURE 10** Craig countercurrent distribution.
EXAMPLE 5 A chromatographic separation.

In Example 5, $V_U$ and $V_L$ are the volumes of the upper and lower phase correspondingly. $f_{A_{p,t}}$ is the fraction of $A$ present in the upper phase in the vessel $p$ after the transfer step $t$, $M_{A_{p,t}}$ is the total amount of $A$ in the vessel $p$ after the transfer step $t$, $K_{A_{p,t}}$ is the equilibration ratio of $A$ in the vessel $p$ after the transfer step $t$. $K_{A_{p,t}}$ can be a constant, but it also can be a function of the total amount $M_{A_{p,t}}$, $M_A$ is the initial amount of $A$ in the separation process. Finally, $K_A$ and $K_A'$ are given constants depending on the component A. $M_{A_p}$ and $M_{A_C}$ are always assumed as given. A consistency analysis of a representative structure shows that, by defining only $V_U$ and $V_L$ as the set of independent variables, the system is structurally consistent for any number of vessels $p$ and transfer steps $t$.

6 SUMMARY

In this paper, we have reviewed the concepts involved in structural analysis. We then derived an extension to Zaher’s consistency analysis of conditional models. This extension allows a consistency analysis to be applied to conditional models in which the number of variables and equations for each of the alternatives may not be the same. In general, we think that, in order to ensure the structural consistency of a conditional model, the combinatorial consistency analysis must be performed. However, we have shown that, by taking advantage of the structure of the problem, it is sometimes possible to reduce the computational effort required by the consistency
analysis. In addition, we used simple examples to illustrate the relevant definitions in structural analysis, to demonstrate the scope of application of the extension to Zaher’s consistency analysis, and to show how we can take advantage of the existence of common incidence patterns and repeated structures in the structural analysis of conditional models.

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8 REFERENCES


APPENDIX A  ELIGIBLE SET FOR A CONDITIONAL MODEL HAVING ALTERNATIVES WITH DIFFERENT INCIDENT VARIABLES

This appendix presents the formal derivation of the eligible set of variables to be used in the consistency analysis of a conditional model when such a conditional model contains alternatives with different incidence sets and different number of equations among them. By using set theory, we show that the set of variables eligible to become independent variables in the context of the overall conditional problem is given by:

\[ e^{k''} = \bigcap_{i}^{s} \left( E^{k}_{i} \cup (M \setminus I_{i}) \right) \]

where \( s \) is the number of the alternative sets of equations, \( e^{k''} \) is the set of eligible variables to be chosen as independent variables for the conditional problem, \( E^{k}_{i} \) is the eligible set of variables to be chosen as independent variables for the alternative \( i \), \( M \) is the maximal set of variables, and \( I_{i} \) is the set of incident variables for the alternative \( i \).

A.1 Notation

Besides the notation already established, the following definitions are used throughout this demonstration.

A.1.1 Set Operators

- \( \text{comp}(A) \) Complement All the elements not in \( A \).
- \( \subset \) Subset \( A \subset B \) means that every element in \( A \) is also contained in \( B \).
- \( \emptyset \) Empty set
- Disjoint Sets \( A \cap B = \emptyset \)
Equal Sets \( A \subseteq B \) and \( B \subseteq A \).

During the derivations, we frequently make use of the Morgan’s Theorem:

\[
\bigcup_j [\text{comp}(A_j)] = \text{comp}[\bigcap_j A_j]
\]

### A.2 Eligible Set in Zaher’s Consistency Analysis

In his work, Zaher (1995) considered the necessary conditions for the structural consistency of a conditional model. He show that, for a conditional model in which all the alternatives have the same incident variables, the eligible set of variables for a conditional model is given by:

\[
e^k = E_1^k \cap E_2^k \cap \ldots E_s^k = \bigcap_j E_j^k
\]  \quad (A.1)

### A.3 Extension of Zaher’s Consistency Analysis to a General Conditional Model

In a general case, the number of equations in each alternative of a conditional model may change and so may the incidence set of variables. This section presents a derivation of the eligible set of a conditional model for that general case.

#### A.3.1 Deriving the Eligible Set in a General Conditional Model

In order to derive the eligible set of variables for a general conditional model, we start by finding the eligible set for each alternative in the context of the overall problem through the following analysis.

Assume that an output assignment performed to each individual alternative results in the eligible sets \( E_i^k \) for an \( i \in \{1 \ldots s\} \). Consider the case of alternative number 1. In order to find the “truly” eligible set of variables for alternative 1 in the context of the overall
conditional model (all the alternatives) we have to eliminate the elements of $E_1^k$ which are ineligible in any of the alternatives. We will denote the resulting corrected set of eligible variables for alternative 1 as $E_1^{k'}$. We obtain:

$$E_1^{k'} = E_1^k \setminus \{ [E_1^k \cap (I_2 \setminus E_2^k)] \cup [E_1^k \cap (I_3 \setminus E_3^k)] \cup \cdots [E_1^k \cap (I_s \setminus E_s^k)] \}$$  \hspace{1cm} (A.2)$$

Here is an explanation of the meaning of (A.2). $(I_2 \setminus E_2^k)$ is the set of variables incident but ineligible to be chosen as independent variables in alternative 2. Hence, $E_1^k \cap (I_2 \setminus E_2^k)$ is the set of eligible variables in alternative 1 which are ineligible in alternative 2. Therefore, $[E_1^k \cap (I_2 \setminus E_2^k)] \cup [E_1^k \cap (I_3 \setminus E_3^k)] \cup \cdots [E_1^k \cap (I_s \setminus E_s^k)]$ represents the set of variables which are eligible in alternative 1 but ineligible in some alternative. With that in mind, the corrected set $E_1^{k'}$ is the set of eligible variables for alternative 1 which can be also considered as eligible in the context of the overall conditional model (note the minus operation in (A.2)).

In general, for any alternative $i \in \{1 \ldots s\}$ the set of eligible variables for each alternative in the context of the overall conditional problem is given by:

$$E_i^{k'} = E_i^k \setminus \left\{ E_i^k \cap \left( \bigcup_{j, \ j \neq i} (I_j \setminus E_j^k) \right) \right\}$$  \hspace{1cm} (A.3)$$

Finally, the union of these individual sets gives the set of eligible variables for the overall conditional problem:

$$e^{k'} = \bigcup_{i} E_i^{k'}$$  \hspace{1cm} (A.4)$$

For a general conditional model, equation (A.4) is the equivalent to equation (A.1) for conditional models in which all the alternatives have the same incident variables.
A.3.2 A simplified Approach

We next show that the previous analysis does not have to be performed as described. We demonstrate that, if we augmented the eligible set of each alternative with the nonincident variables of that alternative,

\[ E_i^{k''} = E_i^k \cup (M \setminus I_i) \]  

and find the intersection of the augmented sets \( E_i^{k''} \),

\[ e^{k''} = \bigcap_i E_i^{k''} = \bigcap_i [E_i^k \cup (M \setminus I_i)] \]

then the resulting set \( e^{k''} \) is completely equivalent to the set \( e^{k'} \) given by (A.4). Recall that \( M \) is the maximal set of variables,

\[ M = I_1 \cup I_2 \cup \ldots I_s = \bigcup_j I_j \]

so that \((M \setminus I_i)\) represents the set of nonincidences in alternative \( i \).

In order to demonstrate our assertion, we first carry out the following derivation. From (A.3), we get,

\[ E_i^{k'} = E_i^k \left\{ E_i^k \cap \left[ \bigcup_{j, j \neq i} (I_j \setminus E_j^k) \right] \right\} \]

\[ E_i^{k'} = E_i^k \left\{ \bigcup_{j, j \neq i} [E_i^k \cap (I_j \setminus E_j^k)] \right\} \]

\[ E_i^{k'} = E_i^k \left\{ \left[ \bigcup_{j, j \neq i} E_i^k \cap (I_j \setminus E_j^k) \right] \cup \emptyset \right\} \]
Then we use (A.9) to obtain,

\[ E^k_i = E^k_i \left( \bigcup_{j, j \neq i} E_i^k \cap (I_j \backslash E_j^k) \right) \cup \left[ E_i^k \cap (I_i \backslash E_i^k) \right] \]

\[ E^k_i = E^k_i \left( \bigcup_{j} E_i^k \cap (I_j \backslash E_j^k) \right) \]

\[ E^k_i = E^k_i \left( \bigcup_{j} [E_i^k \cap (I_j \backslash E_j^k)] \right) \]  \hspace{1cm} (A.9)

Then we use (A.9) to obtain,

\[ E^k_i = E^k_i \left( E_i^k \cap \bigcup_{j} (I_j \backslash E_j^k) \right) \]  \hspace{1cm} (A.10)

\[ E^k_i = E^k_i \left( E_i^k \cap \bigcup_{j} \left( \bigcup_{j} (I_j \cup (M \backslash I_j)) \right) \right) \]

\[ E^k_i = E^k_i \left( E_i^k \cap \bigcup_{j} \left( \bigcup_{j} (M \backslash \left( E_j^k \cup (M \backslash I_j) \right)) \right) \right) \]

\[ E^k_i = E^k_i \left( E_i^k \cap \bigcup_{j} \left( \bigcup_{j} M \backslash (E_j^k \cup (M \backslash I_j)) \right) \right) \]

\[ E^k_i = E^k_i \left( E_i^k \cap \bigcup_{j} M \backslash \left( \bigcap_{j} E_j^k \cup (M \backslash I_j) \right) \right) \]

\[ E^k_i = E^k_i \left( E_i^k \cap \bigcup_{j} M \backslash \left( \bigcap_{j} E_j^k \cup (M \backslash I_j) \right) \right) \]
Thus, by substituting (A.6) in (A.11):

$$E_i^{k'} = E_i^k \cap \left( \bigcap_{j} E_j^k \cup (M \setminus I_j) \right)$$

(A.11)

This is equivalent to:

$$E_i^{k'} = E_i^k \cap \left( \bigcap_{j} E_j^k \cup (M \setminus I_j) \right)$$

(A.12)

and from (A.4):

$$e^{k'} = \bigcup_{i} [E_i^k \cap e^{k''}]$$

(A.13)

which is equivalent to:

$$e^{k'} = \left( \bigcup_{i} E_i^k \right) \cap e^{k''}$$

(A.14)

Finally, since $e^{k''}$ is always a subset of $\left( \bigcup_{i} E_i^k \right)$, we obtain,

$$e_i^{k'} = e^{k''}$$

(A.15)

Q.E.D

(A.15) means that the derivation of the set of eligible variables for a conditional problem presented in A.3.1 can be substituted by the combined use of (A.5) and (A.6).

### A.4 Proof of the Reduction to the Particular Case

We finish our demonstration by showing that both (A.4) and (A.6), reduces to (A.1) when the incidences are the same for all the alternatives.

**A.4.1 Reduction from (A.4)**

Start with equation (A.3)

$$E_i^{k'} = E_i^k \setminus \left( \bigcap_{j, j \neq i} (I_j \setminus E_j^k) \right)$$
since

\[ I_1 = I_2 = \ldots = I_s = I = M \]  \hspace{1cm} (A.16)

then

\[ (I_j \setminus E_j^k) = (I \setminus E_j^k) = (M \setminus E_j^k) = \text{comp}(E_j^k) \]  \hspace{1cm} (A.17)

By using Morgan’s Theorem:

\[ \bigcup_j [\text{comp}(E_j^k)] = \text{comp} \left[ \bigcap_j E_j^k \right] \]  \hspace{1cm} (A.18)

we get the following equivalence:

\[ \bigcup_{j, j \neq i}^s (I_j \setminus E_j^k) = \bigcap_{j, j \neq i}^s (E_j^k) \]  \hspace{1cm} (A.19)

Substituting (A.19) in (A.3):

\[ E_i^{k'} = E_i^k \setminus \left[ E_i^k \bigcap \left[ \bigcap_{j, j \neq i}^s (E_j^k) \right] \right] \]  \hspace{1cm} (A.20)

and further simplifying:

\[ E_i^{k'} = E_i^k \setminus \left[ E_i^k \bigcap \left[ \bigcap_{j, j \neq i}^s (E_j^k) \right] \right] \]  \hspace{1cm} (A.21)

\[ E_i^{k'} = E_i^k \setminus \left[ \bigcap_i (E_j^k) \right] \]  \hspace{1cm} (A.22)

\[ E_i^{k'} = \bigcap_i (E_j^k) \]  \hspace{1cm} (A.23)
From (A.1):

\[ E_{i}^{k'} = e^{k} \]  \hspace{1cm} (A.24)

Finally, from (A.4):

\[ e^{k'} = \bigcup_{i}^{s} E_{i}^{k'} = \bigcup_{i}^{s} e^{k} = e^{k} \]  \hspace{1cm} (A.25)

Q.E.D.

**A.4.2 Reduction from (A.6)**

Starting with (A.5)

\[ E_{i}^{k''} = E_{i}^{k} \cup (M \setminus I_{i}) \]  \hspace{1cm} (A.26)

and since

\[ I_{1} = I_{2} = \ldots = I_{s} = I = M \]  \hspace{1cm} (A.27)

then the set of nonincidences is null for all the alternatives:

\[ M \setminus I_{i} = \emptyset \]  \hspace{1cm} (A.28)

Hence,

\[ E_{i}^{k'''} = E_{i}^{k} \]  \hspace{1cm} (A.29)

and, finally,

\[ e^{k} = \bigcap_{i}^{s} E_{i}^{k} = \bigcap_{i}^{s} E_{i}^{k'''} = e^{k'''} \]  \hspace{1cm} (A.30)

Q.E.D.