Proceedings of the 2011 4th International Symposium on Advanced Control of Industrial Processes, Thousand Islands Lake, Hangzhou, P.R. China, May 23-26, 2011, pp 15-21

Merging Process Models and Plant Topology

G.J. Di Geronimo Gil, D.B. Alabi, O.E. Iyun, and N.F. Thornhill *Senior Member, IEEE*

***Abstract*— The paper discusses the merging of first principles process models with plant topology derived in an automated way from a process drawing. The resulting structural models should make it easier for a range of methods from the literature to be applied to industrial-scale problems in process operation and design.**

Keywords: Connectivity matrix; fault detection and diagnosis, plantwide disturbance; plant topology; root cause; XML.

I. Introduction

THIS paper assesses the potential for the integration of plant topology information[1] from process drawings such as process flow diagrams with information derived from first principles process models. It considers specifically the generation of models of the *structure* of a process. Such models are typically represented as a digraphs or, equivalently, as a matrix. The purpose of such a model is to capture cause-effect relationships between the items or variables in the graph.

An aim of merging process models and plant topology is to enable engineers to combine information from disparate sources in order to make inferences that will improve the operation of a plant. The key step is a formal representation of the elements and parts of a process and the relationships between them. The automated capture of connectivity and plant topology from process diagrams marks a major step forward in the possibilities for industrial implementation of methods from the literature that have to date been constrained by the need to construct the connectivity representation manually. On the other hand, the information held in the process drawing is limited to items of equipment and the connections between them. Such a representation does not capture the relationships between the variables that describe the physics and chemistry of the process. A means to automatically generate a structural model capturing the first principles relationships would be very useful, It would open up existing applications for large-scale implementation and generate a platform for new applications.

Manuscript received January 31st 2011.

Alabi, Di Geronimo Gil and Iyun are graduate students in the Centre for Process Systems Engineering, Department of Chemical Engineering, Imperial College London. Di Geronimo Gil gratefully acknowledges the award of a Commonwealth Scholarship. N.F. Thornhill holds the ABB/RAEng Chair of Process Automation in the Department of Chemical Engineering, Imperial College London, London SW7 2AZ (n.thornhill@imperial.ac.uk).

[1] The term topology is used here in its definition as the physical structure of a network.

Figure 1 shows relevant literature discussing first principles structural models (upper left) and topology-based structural models from P&IDs (lower left). When these are combined (black box, centre) many applications become possible, as shown on the right hand side of the figure.

The paper starts with an overview of structural modeling of chemical processes. It then gives an account of work-in-progress towards automated structural modeling to generate first principles structural relationships starting from a process drawing. It also outlines briefly a new application in automated analysis of control degrees of freedom which then becomes possible.

II. Structural Process Models

Structural representation is a decomposition of a model to show the relationships between the items or variables in the model without the need for accurate values of the actual parameters of the system. The structural representation can identify causality, can predict propagation of events and give insight into the characteristics of the model and the causal relationships in the system.

A *first principles structural model* captures the mathematical structure of a system. For instance it would show a causal link between the temperatures of the exit steams from a heat exchanger and the inlet temperatures and the flow rates, but without providing the detailed equations that enable determination of the exit temperatures. It is typically represented in the form of a digraph, or a signed digraph if the positive or negative directions of the influences are known. An equivalent representation is a variable relationship matrix which represents the arcs of a digraph as 1's, where the rows and columns of the matrix represent the nodes of the digraph.

Many of the applications and analysis methods on the right hand side of Figure 1 require an input in the form of a first principles structural model of the process. Getting this input in place is a bottleneck, however, especially for a large scale plant-wide applications.

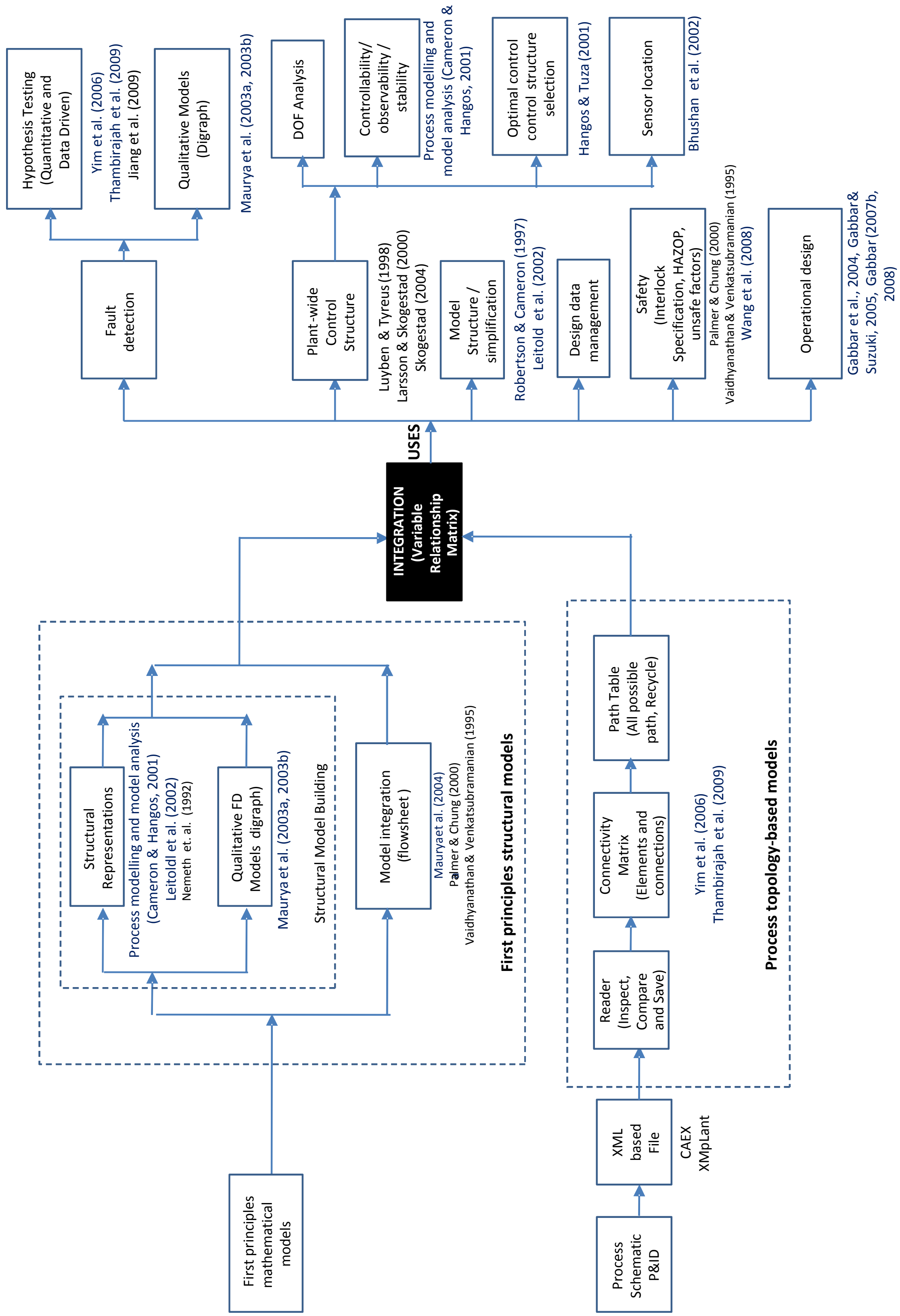

Fig.1. Literature relevant to structural process models and their applications

The model generated from a process flow diagram (PFD) or piping and instrumentation diagram (P&ID) is typically different in its nature from that generated from a first principles model. The reason is that the PFD and P&ID describe items of equipment, instruments and pipes. The causal relationships between them may be inferred from the physical layout of the plant, and in particular the directions of flow are important. Models that describe the plant connectivity are referred to as *topology-based models* or *process connectivity models*. A strong motivation for using topology-based models as a front end for the applications of Figure 1 is the wide availability of computer generated drawings for industrial scale processes. If these can be utilized, then it removes the bottleneck of getting the plant information into the applications.

A topology-based model derived from a PFD or P&ID shows items of equipment and the directional connections between them, but there is not always enough information for analysis. For instance, a disturbance in feed composition not be deduced from the P&ID as the cause of upset temperatures in a separation column unless the drawing happened to show a composition sensor. Therefore it is useful to link information about variables such as temperature, composition, pressure and flow rate with connectivity models to enhance the cause-effect representation of the process.

By contrast, a first principles structural model shows relationships between these variables that describe the process behaviour. The challenge is to start with the process drawing and to end up with a first principles structural model.

A. Topology based models

An example of a basic topology-based model is shown in Figure 2 which shows the connectivity between the items of equipment in a chemical plant. The model is in the form of a connectivity matrix showing directional connections between the main items of equipment. The row headings are the items of equipment from which a process flow originates, and the column headings show the destinations of the flow. The entry 1 on the right and four rows from the bottom shows, for instance, that a flow exists from mixer-001 to reactor-001. However, there is no flow from reactor-001 to mixer-001 because there is a 0 in the intersection of the row headed reactor-001 and the column headed mixer-001.

This connectivity matrix was generated automatically by co-authors Iyun and Alabi from a PFD drawn with a CAD tool. With such a simple case it is also feasible to create the matrix by hand. However, other examples in later sections of this paper show the task would rapidly become unmanageable at larger scales.

	SPLITTER-002	REBOILER-001	SEPARATOR-001	SPLITTER-001	COMPRESSOR-001	MIXER-001	STRIPPER-001	CONDENSER-001	REACTOR-001
SPLITTER-002		1							
REBOILER-001							1		
SEPARATOR-001				1			1		
SPLITTER-001					1				
COMPRESSOR-001						1			
MIXER-001									1
STRIPPER-001	1					1			
CONDENSER-001			1						
REACTOR-001								1	

Fig 2. A simple topology-based model in the form of a directional connectivity matrix.

The process industries use Standards IEC/PAS 62424, ISO 10303-221 and ISO 15926 which enable exchange of engineering data. They export a description of the drawing and the items in it in machine readable electronic form. XML is used to provide a common format for the data exchange, for instance between CAD tools and the engineering tools for design of the automation system. Intelligent computer-aided drawing tools for export and exchange of process drawings and P&IDs include Aveva's VPE P&ID, Comos P&ID from Siemens and SmartPlant P&ID from Intergraph.

The structure of the XML file is governed by a schema. The XML export from a P&ID drawn in an ISO 15926 CAD tool conforms with the XMpLant schema, while CAEX is an XML schema for the export from an IEC/PAS 62424 compliant CAD system. These have been described elsewhere [1-4].

Yim *et. al*. [3] and Thambirajah *et. al*. [4] developed a tool to parse and extract the connectivity information form an XML file using the CAEX schema. The examples presented in this papers use ISO 15926 and XMpLant.

B. First principles structural models.

The review papers of Venkatasubramanian *et al*. [5-7] presented a classification of methods for analysis of process operations into quantitative model-based methods, qualitative model-based and process history based methods. Qualitative methods allow the introduction of first principles information into a model even in the absence of quantitative information. For instance, they can show that pressure and temperature are related in a gas because an equation of state exists, but without specifying the equation of state. As discussed earlier, a first principles structural model in the form of a directed graph (digraph) provides a causal structure. A number of authors have contributed work in the area first principles structural modeling, as indicated in the top left hand side of Figure 1.

III. INTEGRATION OF STRUCTURAL MODELS

The linkage between topology-based models and first principles structural models may be made by storing simple structural models of basic units such as heat exchangers, reactors and separation units in a library. When one of these units is identified in the process topology, a relevant model is extracted from the library. It is connected with models of other units according to the topology indicated in the topology-based model.

Previous work related to the construction of structural representation of models for flowsheets includes Vaidhyanathan and Venkatsubramanian [8], Palmer and Chung [9], and Maurya *et al*. [10,11]. All of them suggest the integration of individual models for each plant element as the procedure to create plantwide structural models.

As an illustration of the linking of plant topology with process models, an automated front end to Case Study 2 from Maurya *et.al*. [10] has been developed by co-author Di Geronimo Gil. Figures 3 and 4 show the process flow diagram and the topology-based connectivity matrix that was extracted automatically from a computer-aided drawing of the PFD by co-authors Iyun and Di Geronimo Gil.

The key challenge in generation of a first principles structural model from a plant topology model is to assign physical variables and equations to the plant items that are in the topology-based connectivity matrix. The biadjacency matrix of Maurya *et.al*. [10] is the heart of the method and once it is in place the methods of perfect matching also described in their paper may be applied to the plantwide biadjacency matrix to construct the variable relationship connectivity matrix which is the first principles structural model. A biadjacency matrix shows model equations as row headings and variables as column headings. The presence of a 1 in a cell of the matrix associates a variable with an equation. *Perfect matching* is a means of deciding which variable in an equation will be considered the dependent variable. Perfect matching means that each model equation is associated with just one dependent variable. It finds a structure in the equations such that each equation allows the determination of one of the system variables from the others.

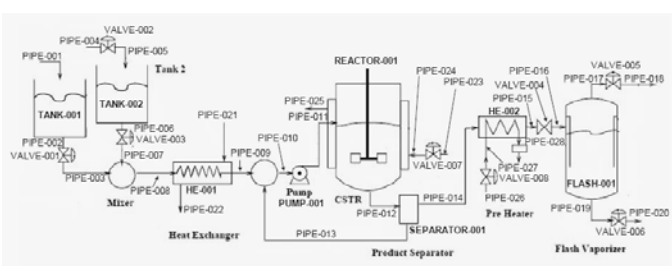

Fig. 3. Case study process from [10]

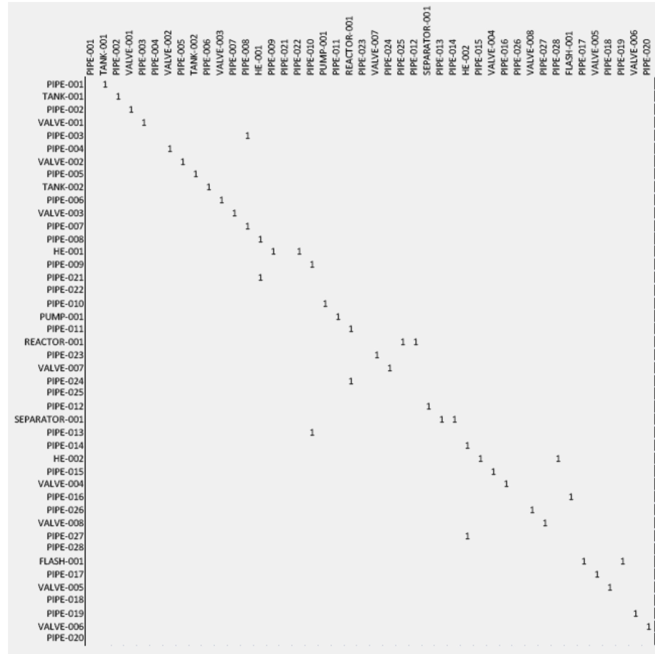

Fig. 4. Topology-based model for the case study from [10]

The following functionality was coded in a DotNet Windows application by author Di Geronimo Gil:

- A facility to create a connectivity matrix or to introduce it from other application. This matrix is used as input for the generation of the plantwide biadjacency matrices.
- A library to store the individual biadjacency matrices for the individual models corresponding to the elements commonly appearing in the flowsheet. The library interface includes facilities to upload new elements in the library and modify the existing ones.
- A function to integrate the biadjacency matrices of individual elements according to the information extracted from the connectivity matrix and to build a biadjacency matrix for the whole process.
- A method for solving the perfect matching problem for the plantwide biadjacency matrix.
- A function to construct the variable relationship connectivity matrix from the perfect matching and the plantwide biadjacency matrix.

Generic models from different unit operations were developed and stored in the library. This step provides the mechanism by which the physical variables of the process are brought into the description outlined by the process topology.

Each individual model was connected using the connectivity information from the plant topology by matching outlet variables of the upstream connected elements to the input variables of the downstream element. An example is shown in Figure 5 where the equations in the centre show the matching.

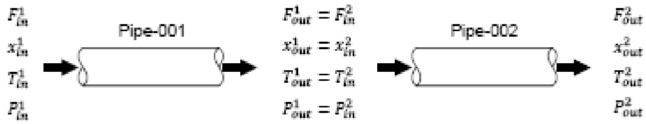

Fig. 5. Example showing how models are connected

	Pipe-001.Fin	Pipe-001.xin	Pipe-001.Tin	Pipe-001.Pin	Pipe-001.Fout	Pipe-001.xout	Pipe-001.Tout	Pipe-001.Pout	Valve-001.Fin	Valve-001.xin	Valve-001.Tin	Valve-001.Pin	Valve-001.S	Valve-001.Fout	Valve-001.xout	Valve-001.Tout	Valve-001.Pout	Pipe-002.Fin	Pipe-002.xin	Pipe-002.Tin	Pipe-002.Pin	Pipe-002.Fout	Pipe-002.xout	Pipe-002.Tout	Pipe-002.Pout
Pipe-001.Eq1	1				1																				
Pipe-001.Eq2		1				1																			
Pipe-001.Eq3		1	1	1	1			1																	
Pipe-001.Eq4			1				1																		
Pipe-001.Valve-001.F					1				1																
Pipe-001.Valve-001.xi						1				1															
Pipe-001.Valve-001.T							1				1														
Pipe-001.Valve-001.P								1				1													
Valve-001.Eq1									1					1											
Valve-001.Eq2										1					1										
Valve-001.Eq3												1	1	1			1								
Valve-001.Eq4										1	1	1				1	1								
Valve-001.Pipe-002.F														1				1							
Valve-001.Pipe-002.xi															1				1						
Valve-001.Pipe-002.T																1				1					
Valve-001.Pipe-002.P																	1				1				
Pipe-002.Eq1																		1				1			
Pipe-002.Eq2																			1				1		
Pipe-002.Eq3																			1	1	1	1			1
Pipe-002.Eq4																				1				1	

Fig. 6. Biadjacency matrix example

Figure 6 is part of a biadjacency matrix generated automatically by the application. It shows model equations as row headings and variables as column headings, and the grey sections are plant sections identified from the process drawing.

The biadjacency matrix is an input into the perfect matching procedure devised in [10]. Simple cases can be solved by manipulation of the entries of the biadjacency matrix, while more complicated cases are solved as an optimization problem. The end point is a matrix representation similar to the biadjacency matrix but with a one-to-one match between variables and equations i.e. only one entry in each row.

The automation of this stage of the work is still in progress. At the time of writing it uses a manual step by which the biadjacency matrix is transferred electronically as an input to GAMS to generate the perfectly matched matrix.

Finally, as explained in [10], the perfect matching as generated by GAMS and the biadjacency matrix are combined to construct the variable relationship connectivity matrix, which constitutes the first principles structural model. The model is much larger than the original topology-based model because each plant element has several variables associated with it. The resulting model is shown in Figure 9 at the end of the paper.

IV. Application to Degrees of Freedom Analysis

Export of process topology from a PFD can help in obtaining the control degrees of freedom which would be a useful tool during the design of a new plant. The example application is the control of the plant from Luyben *et. al*, [12] whose process flow diagram is shown in Figure 7. It is known that this process has 26 control degrees of freedom. The drawing and a topology-based model were generated by co-authors Alabi and Iyun. The automated degrees of freedom analysis was based on the work of [13] and [14]. The result of this method is that control degrees of freedom is the total number of material and energy streams in a process minus the total number of steady state material balances, referred to as restraining number in the work by Konda *et, a*l. [15].

The total number of streams is easily determined by counting the number of 1 entries in the topology-based model of the PFD, plus the feed and product streams. Steady state balances are determined in a way similar to the approach described in Section IV.(A) by matching elements in the drawing against a library of models.

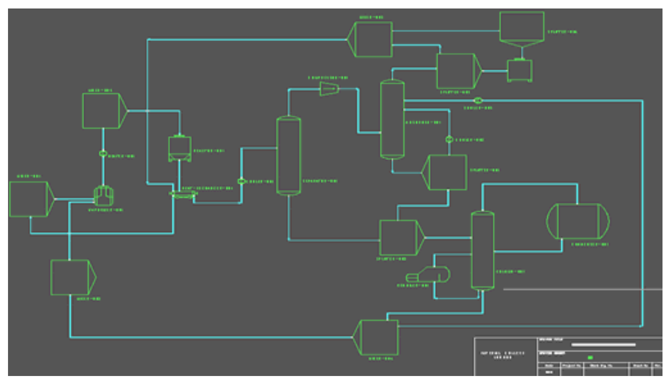
Fig. 7. PFD for the vinyal acetate proces of Luyben [12]

	HEAT-EXCHANGER-1	COOLER-1	SEPARATOR-1	COMPRESSOR-1	ABSORBER-1	MIXER-1	SPLITTER-1	COOLER-2	SPLITTER-2	COLUMN-1	REBOILER-1	MIXER-4	MIXER-2	SPLITTER-3	MIXER-5	CO2-REMOVAL-1	SPLITTER-4	CONDENSER-1	VAPORIZER-1	HEATER-1	MIXER-3	REACTOR-1	COOLER-3
HEAT-EXCHANGER-1		1				1																	
COOLER-1			1																				
SEPARATOR-1				1					1														
COMPRESSOR-1					1																		
ABSORBER-1							1							1									
MIXER-1																			1				
SPLITTER-1								1	1														
COOLER-2					1																		
SPLITTER-2										1													
COLUMN-1											1	1						1					
REBOILER-1										1													
MIXER-4													1										1
MIXER-2																			1				
SPLITTER-3															1	1							
MIXER-5	1																						
CO2-REMOVAL-1																	1						
SPLITTER-4															1								
CONDENSER-1										1													
VAPORIZER-1																				1			
HEATER-1																					1		
MIXER-3																						1	
REACTOR-1	1																						
COOLER-3					1																		

Fig. 8. Topogy-based connectivity model for the process in Fig 7.

V. SUMMARY

This article has shown that it is possible and timely to link first principles models for individual items of process equipment with process topology information extracted directly from process drawings (PFDs or P&IDs). It demonstrated examples of topology-based models in the form of a process connectivity matrix extracted from drawings. The paper demonstrated it is possible to augment the topology-based model with information from first principles modelling. This enables a first principles structural model of a process to be generated from the process drawings that are routinely used during process design. Both the topology-based model and the first principles structural model provide a useful front end to a number of potential applications from the literature, many of which have until now been constrained by the bottleneck of having to prepare the structural models by hand.

VI. LIST OF CITED PAPERS

The papers in Fig. 1 not cited in the main text are listed here. They are: Cameron and Hangos [16]; Leitold *et.al*. [17]; Nemeth *et.al*. [18]; Maurya *et.al*. [19]; Luyben and Tyreus [20]; Larsson and Skogestad [21]; Skogestad [22]; Robertson and Cameron [23]; Wang et.al [24]; Gabbar *et.al*. [25]; Gabbar and Suzuki [26]; Gabbar [27,28], Jiang *et.al*. [29]; Hangos and Tuza [30]; Bhushan *et.al*. [31].

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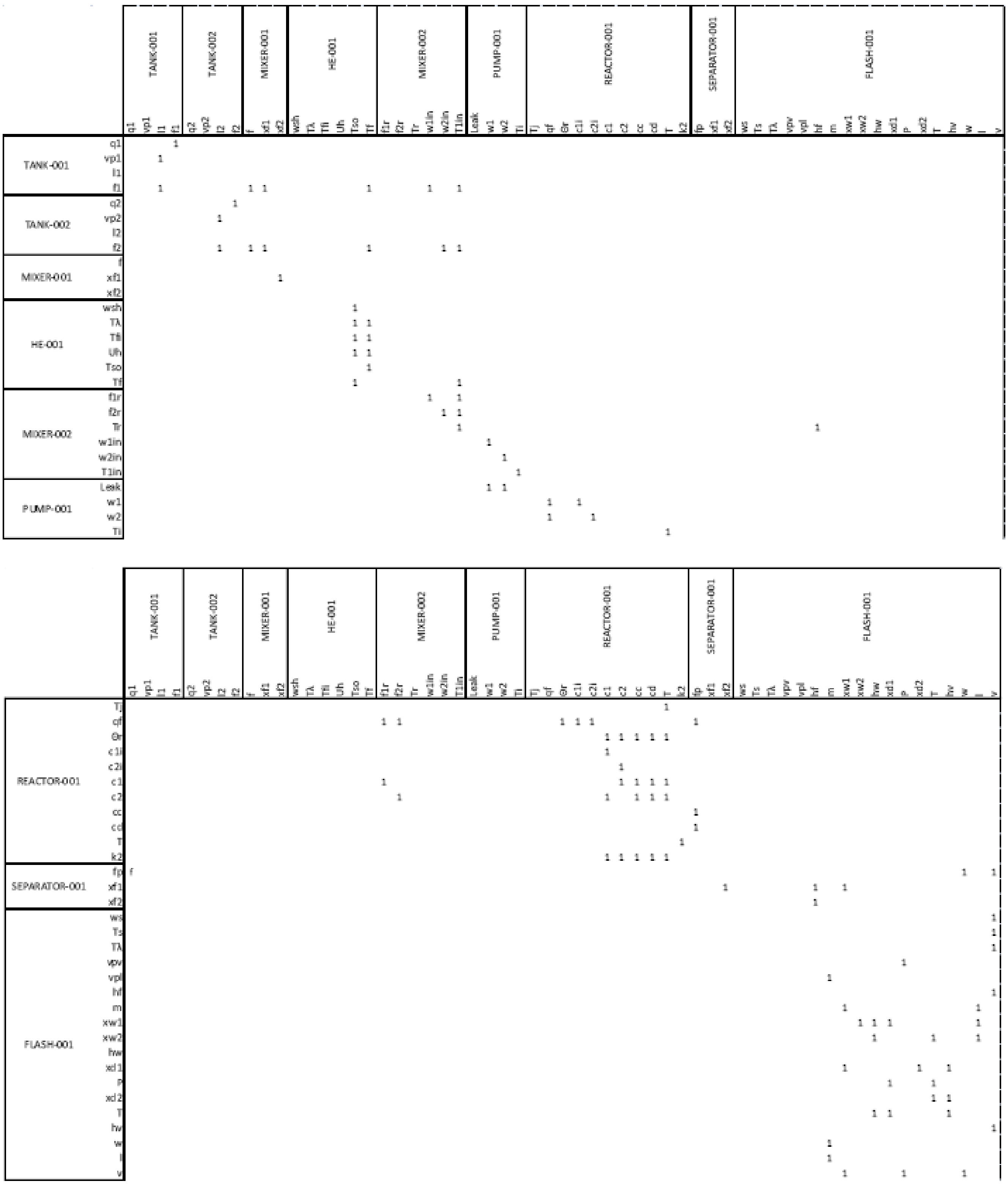

Fig. 9. First principles structural models for the case study from [10]