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Published in:
Chemical engineering transactions

Link to article, DOI:
[10.3303/CET1870014](https://doi.org/10.3303/CET1870014)

Publication date:
2018

Document Version
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

Citation (APA):
Restrepo, J. B., Forero, H. A., & Cardona, C. A. (2018). The analysis of chemical engineering process plants and their models represented by networks. *Chemical engineering transactions*, 70, 79-84.
<https://doi.org/10.3303/CET1870014>

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The Analysis of Chemical Engineering Process Plants and their Models Represented by Networks

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Chemical process plants can be interpreted as networks where energy mass and momentum are exchanged. Therefore, they can be represented as such using graph theory. This work presents a decomposition methodology that allows to conceptually deconstruct chemical process plants and their models to be represented by networks. By the selection of minimum constituent units of the plant, it is possible to describe the interdependencies among those minimum units. This procedure allows the correct representation of process plants as networks along with a detailed analysis of them. Using network metrics such as centrality measures, it was possible to analyze, as an example, the HDA process plant under two selected plantwide control strategies, allowing the identification of its more important units and controllers. This permitted an insight of how plantwide control strategies responded to perturbations from a qualitative point of view. It was also possible to establish the main coincidences and discrepancies between the selected plantwide control strategies.

1. Introduction

In the design and optimization of a chemical process plant, the main objective is to couple the different plant units to interact as much as possible in order to achieve the desired production and environmental goal (El-Halwagi, 2012). While in the control system design, the main objective is to deal with unit to unit undesired interactions, by designing a control system that counteracts disturbances before they propagate from their source to other units (de Araujo et al., 2007). Along with data analysis of process plants, models have played a fundamental role in the design and control of processes. Once the desired model is constructed, its qualitative and quantitative analysis is not always simple. Process models are mathematically (non-linear) and structurally (a big number of components) complex. Nevertheless, the representation of chemical process models as networks can be useful. In general terms, a network is any system that admits an abstract mathematical representation as a graph. Nodes (vertices) identify the elements of the system and in which the set of connecting links (edges) represent the presence of a relation or interaction among those elements. Clearly, such a high level of abstraction generally applies to a wide array of systems (Barrat et al., 2008).

Networks have been used widely for many applications in diverse fields of chemical engineering, such as dynamic process modelling (Mangold *et al.*, 2005), diagnosis and fault detection (Zhang and Hoo, 2011), plantwide analysis (Preisig, 2009), process synthesis (Friedler et al., 1995), complex system study (Elnashaie and Grace, 2007), just to name a few.

The extensive work on graphs in different application fields and especially on chemical engineering has motivated the adaptation and use of the methodology proposed by Gilles (1998) and Mangold et al. (2002) for the decomposition of process plants and their models, into control volume graphs. With the main purpose of obtaining representative graphs of process models that can be qualitatively analysed to infer non-trivial properties with the aid of network analysis, which is a well-established and quickly evolving discipline.

2. From models to graphs

Any model needs a reference point, and the control volume provides it. A control volume is a defined region of three dimensional space, which has an associated Volume V and surface S (Hangos and Cameron, 2001). A control volume contains a static or moving fluid that interacts with everything outside itself through the control Surface S .

For a model to be suitable to be represented as a network, it must be a deterministic model. A deterministic model represents the view of the modeler of the plant; it describes the containment of and the interactions between the different internal structural elements (Westerweele, 2003). The following identification steps are proposed as the first step to generate a graph from a chemical process and its process model.

- **The scope of the Model:** The first step in the deconstruction and representation process would be to identify the scope of the model. The scope of the model will help to understand what is relevant to the model and will be a useful tool to discern what should be used in the construction of the graph and what not.
- **Boundaries:** Once the scope of the model is identified, the next step is to identify the models boundaries, and to clarify which elements are inside and which elements are outside those boundaries (i.e., the environment or surroundings) or interact with elements outside those boundaries (e.g., convective flows coming from non-modelled units).
- **Control Volumes:** Once the global boundaries of the model are clear, the next step would be to identify the internal boundaries of the model. Those internal boundaries, in this case, would be the modelled control volumes and the connection elements. Connection elements are elements that define the magnitude and direction of the flow of mass, energy, and momentum, elements such as pumps, compressors, valves, and weirs. A special case of connection element would be the boundary condition in a distributed parameter system.
- **Flows and dependencies:** The last step would be to determine the state dependencies and direction of the mass, energy, and momentum convective and diffusive flows.

Once each of the components and their relations are identified according to the above-mentioned steps, the last step is to assign each component the appropriate nodes and then depending on the kind of relation identified, to state these relations by means of edges, straight edges for material, energy, and momentum flows; and curved edges to indicate state dependencies. This methodology is represented in Figure 1.

For the case of distributed parameter models, which as their name suggests, incorporate the spatial variation of states within the control volume. They account for situations where the scalar field of the intensive quantities is both a function of time and position (Hangos and Cameron, 2001). These systems are described by partial differential equations (PDEs) or partial differential algebraic equations (PDAEs). The application of conservation principles to distributed parameter systems is based on the selection of a differential control volume. A distributed parameter model can be understood theoretically as an infinite succession of differential control volumes. In practice, it can be understood as a finite succession of finite control volumes along the spatial coordinates, e.g., a Plug Flow Reactor can be approximated by a succession of Continuous Stirred Tank Reactors.

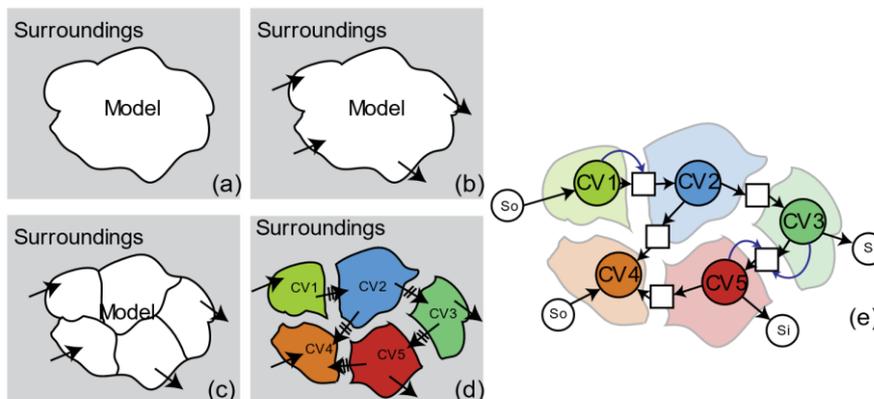


Figure 1. Steps for model deconstruction into graphs a) The model and its Surroundings b) material, energy, and information across the control surface c) Dividing the model into its constitutive control volumes d) Stating the flows between the control volumes e) Generating the graph.

3. Network analysis

Complex network theory (Boccaletti et al., 2006) provides important tools to understand the role and importance of certain nodes within a specific network. Centrality measures (Koschützki et al., 2005) quantify the importance of certain nodes in a network. They have been widely used in diverse fields of application such as the study of AIDS (Borgatti, 1995), Neurology (Rubinov and Sporns, 2010), and Electrical network vulnerability (Wang et al., 2010). The value of these centrality measures is that they can be applied to a wide number of real world systems modeled as networks, where information, matter, and energy or electricity are flowing through. Some of these measures make implicit assumptions about the way information flows through a network. Therefore, it is important to clarify which are those assumptions and when are they relevant to a certain purpose.

3.1 Degree centrality ($C_D(i)$)

The degree k_i of a vertex i is the number of edges in the graph incident on that vertex. For directed graphs the in-degree ($k_{i,in}$) of the vertex i is the number of edges arriving at i . While its out-degree ($k_{i,out}$) is the number of edges departing from i . The degree centrality can be interpreted as a measure of immediate effects. In the eventual case of a failure, nodes with a higher degree will be affected faster than nodes with a lower degree.

3.2 Closeness Centrality ($C_C(i)$)

The closeness centrality of a vertex i expresses the average distance of a vertex (measured by shortest paths) to all others. It becomes an index of the probability that given a perturbation on a node j chosen randomly, the node i will be reached first.

3.3 Betweenness centrality ($C_B(i)$)

The Betweenness centrality (Freeman, 1979) is the number of shortest paths between pairs of vertices that pass-through a given vertex. Betweenness is conventionally thought to measure the volume of traffic moving from each node to every other node that would pass through a given node. Thus, it measures the amount of network flow that a given node controls (Borgatti, 2005)

4. Case study: analysis of the HDA process with plantwide control

The HDA process as described in Douglas (1988) contains a reactor, a furnace, a vapor-liquid separator, a recycle compressor, two heat exchangers, and three distillation columns. Two raw materials, hydrogen, and toluene are converted into the benzene product, with methane and diphenyl as byproducts. The HDA plant is non-linear, large scale, relative degree zero process, highly integrated and non-minimum phase (Herrmann et al., 2003). Therefore, it has been a testing bed of new methodologies of plantwide control.

4.1 HDA Plantwide Control proposed by Luyben et al. (1998)

In this plantwide control strategy, the control variables were chosen to control the inventory of all the components present in the process. The Hydrogen inventory is controlled by the pressure control of the recycle gas loop. The Methane inventory is controlled by the composition control of the recycle gas loop. The benzene inventory is controlled by the temperature control in the benzene column. The toluene inventory is controlled by the level control in the reflux drum of the toluene column. The diphenyl inventory is controlled by the temperature control in the toluene column. Besides the inventory control, other regulatory control loops are present and can be seen in Figure 2a.

4.2 HDA Plantwide Control proposed by de Araujo et al. (2007a, 2007b)

The objective of this plantwide control strategy is to achieve a self-optimizing control, where fixing the primarily controlled variables at constant set points indirectly leads to near-optimal operation. Flow control of the hydrogen feed rate, reactor inlet pressure with purge flow, flow control of the toluene feed rate, quencher outlet temperature with cooling flow from the separator; reactor inlet temperature with furnace heat duty, separator level using its liquid outlet flow rate to the distillation section (Figure 2b). A detailed discussion of the supervisory control layer can be found in de Araujo et al. (2007b).

5. Graph analysis

Complex Networks (Figure 3) are obtained once both plantwide control schemes in Figure 2, are deconstructed into their constitutive control volumes with the considerations made in section 2. Each distillation column was modeled as an equilibrium stage operation which is deconstructed as a succession of control volume nodes (the trays) which are intermediated by flow restriction non-capacitive nodes (the weirs). The reactor was modelled as a succession of finite control volume nodes connected by weighted edges that add up to the residence time. Each controller is modeled as an information node, as each controller is assumed to be a Proportional Integral Derivative Controller (PID), they are interpreted as information capacitances. Heat exchangers, flash drums, distillation sumps and reflux tanks were all divided and represented as control volume nodes. All those deconstructed units together compose the graphs obtained Figure 3.

Table 1. Metrics of the generated graphs

Metric	Value	Value
Number of nodes	209	204
Number of links	407	397
Avg. Node degree	1.95	1.95
Avg. Path Length	21.69	19.78
No. Shortest paths	39412	38210
In degree γ	2.07	2.08
Out Degree γ	2.11	2.12

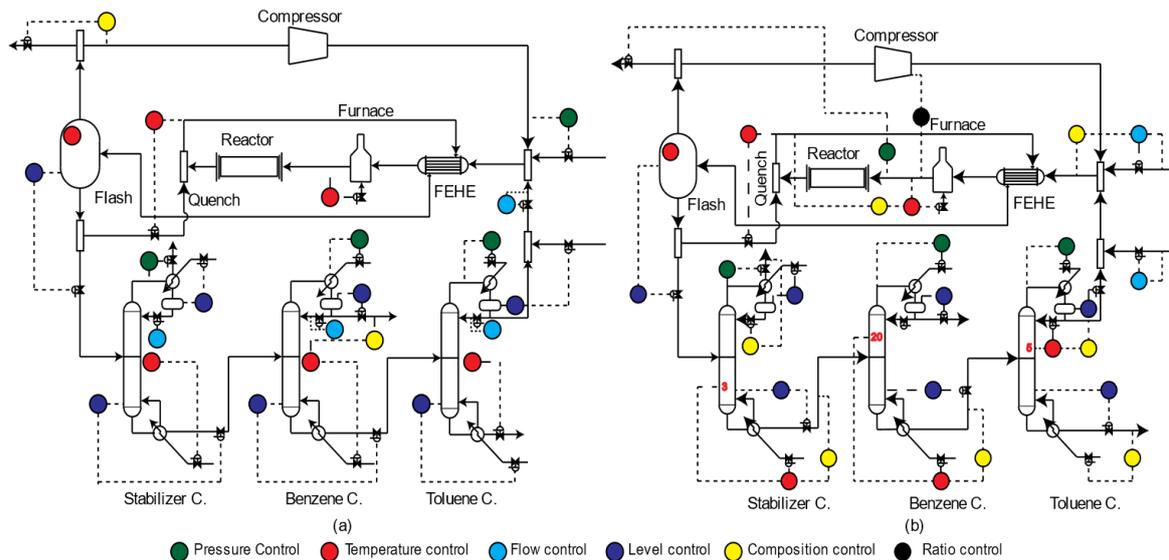


Figure 2. a) HDA plant with plantwide control proposed by Luyben et al. (1998) b) HDA plant with plantwide control proposed by de Araujo et al. (2007)

5.1 Degree centrality analysis

Using the techniques proposed in (Clauset et al., 2009), it was possible to obtain the scaling parameter (γ) for the in and out degree distributions (See Table 1). Many real-world networks such as the World Wide Web (WWW), the internet, social networks, citation networks and food webs; also adjust well to the power law ($P(k) = k^{-\gamma}$) with $2 \leq \gamma \leq 3$ (Barabási, 2009). They are called scale free networks.

5.2 Closeness centrality analysis

When a plantwide control strategy is applied, controllers are added with the aim of maintaining certain process variables in desired values. In other words, a response system to perturbations is implemented. As stated before closeness centrality can be interpreted as an index of the expected time until the arrival of something flowing through the network. Although perturbations tend to propagate in multiple directions at the same time, for a short term after the perturbation, the use of the shortest path will suffice for the analysis (a similar assumption was made and proven true in Maurya et al. (2003)).

In Luyben et al. (1998) control strategy, the most central node is the level controller in the reflux tank of the toluene column, followed by the temperature controller of the furnace and the reflux pressure controller in the inlet mixer. As this strategy focuses on inventory control, the high centrality of this controllers shows that the probable initial response to random perturbations will be to maintain the toluene and hydrogen inventories. In de Araujo et al. (2007a, b) the most central controllers are located in the rectifying section of the benzene column, in the reactor section and in the top of the toluene column. The control strategies are centered on the probable first response on reaction efficiency, which is congruent with the economic analysis presented in de Araujo et al. (2007a).

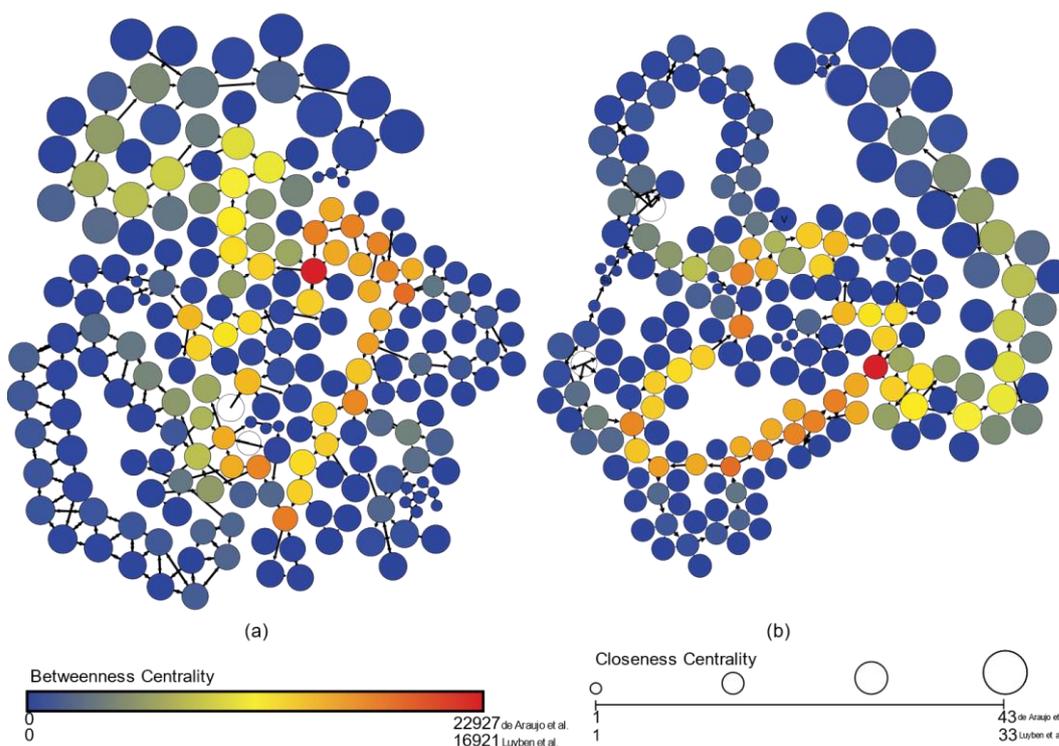


Figure 3. Complex Networks Closeness and Betweenness Analysis (a) de Araujo et al. (2007b, a) (b) Luyben et al. (1998)

5.3 Betweenness centrality analysis

As described before, the betweenness centrality of a node can be interpreted as the measure of the amount of network flow that a given node controls. For both strategies, most of the important controllers are in the product recovery section. Meaning that both plantwide strategies give high importance to product recovery and that two different control philosophies converge on the same objective. Araujo et al. (2007b, a) control scheme has important controllers in the reactor section with high betweenness centrality values, while Luyben et al. (1998) has only one. These results show that the de Araujo et al. (2007b, a) plantwide strategy is more balanced between the product purity control and the reaction zone control.

6. Conclusions

Two plantwide control strategies from representative authors in chemical engineering control were chosen to be analyzed. To do so, the HDA plant was deconstructed using the proposed methodology, and network metrics were applied to infer important properties of both strategies and of the plant itself. The first representative result was the characterization of the resulting networks as scale free. Scale free networks have the property of being robust against random failures but vulnerable to intentional attacks. Another important network property identified was that the average shortest path length is high, discarding this network as a small world network. This centrality measure allowed the identification of the reactor as the most important unit in the plant, the one that will be ultimately affected by anything that happens in the plant. The centrality analysis of both plantwide

control strategies can be used to formulate a methodology of inspection and controller maintenance, aimed toward the correct distribution of efforts to assure the correct functioning of the plant.

The use of network analysis to qualitatively and quantitatively analyze process plants and process models is still in development. There are still many challenges to face such as the correct linking between the simulation and the network representations to obtain better results. Nevertheless, it is a promising analysis methodology that has given important results, and its study would bring important advances to engineering in general.

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