The Complex Topology of Chemical Plants

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Abstract

We show that flowsheets of oil refineries can be associated to complex network topologies that are scale-free, display small-world effect and possess hierarchical organization. The emergence of these properties from such man-made networks is explained as a consequence of the currently used principles for process design, which include heuristics as well as algorithmic techniques. We expect these results to be valid for chemical plants of different types and capacities.

Key words: Scale-free networks, Small-world networks, Chemical plants
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Several systems in nature and human society are constituted by a large number of interacting agents that form a network with complex geometry exhibiting small-world, scale-free and hierarchical features (1; 2). Examples include many of the existing metabolic processes (3), food webs (4), and the relations in social groups (5). An important aspect always present in these systems is a self-regulatory behavior that is responsible for their robustness to perturbations and flexibility to respond to environmental changes and external stimulus. Such a relation between robustness and flexibility, that represents a necessary ingredient to ensure and maintain the functionality of the system, generally results from the fact that the global organization of agents is reached in the absence of any central control, but as a collective phenomenon emerging from

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local interactions. In this way, the generation of a decentralized structure prevents the occurrence of those vulnerable points where an attack could lead to the overall collapse of the network (6). At the same time, this non-central feature makes the complex system more adaptable, because it allows for the local response of agents to the variability of external conditions and eventual specific demands.

An obvious question arising from these facts and ideas that is far from being answered is how local interactions among elementary units of the network can naturally generate a dynamics with global organization. At present, the study of these complex systems depends on the development of new techniques to elucidate their behavior by (*i*) analysing the topological structure of their network of interactions, and (*ii*) investigating the origin and characteristics of their intrinsic self-organized dynamics. The interplay between these two elements, namely, topology and dynamics, can be very effective in revealing the mechanisms behind the regulatory strategies of real systems in nature. Furthermore, this could lead to novel ideas for design of artificial networks with improved performance that display small-world and/or scale-free properties like, for instance, the network of electrical energy distribution (7) and the Internet (8).

In many ways, a chemical plant can be considered as a complex system whose dynamics has to follow very strict conditions of robustness and, on the other hand, to operate with certain flexibility. Specifically, the project of a chemical process is the result of an enterprise decision supported by a strategic plan to attend the market of a region and generate profit. In the case of an oil refinery, for example, this type of industry must be able to provide a broad spectrum of chemicals that are produced at large amounts, but obeying very strict specifications within a productive process that can also be very peculiar in terms of safety and environmental impact. The design of a chemical plant certainly represents one of the most intricate and creative engineering activities (9). A task that is usually performed by chemical engineers, it requires a detailed knowledge of the thermodynamics and transport phenomena taking place at the level of each unitary operation that constitutes the system. Furthermore, the designer must have a sufficiently integrated view of the process to succeed in the development of its complex flowsheet and selection of operational conditions, with also enhanced performance in terms of selectivity and cost of the desired product.

Finally, it is of paramount importance to mention that the accomplishment of a project for a chemical process is surely not a one-to-one task, i.e., two effective solutions obtained from different design teams might be substantially different. In order to overcome the great complexity and expedite the development of the process flowsheet, some *reasonable choices* have to be made that are not formally based on mathematical or physical principles. Indeed, this

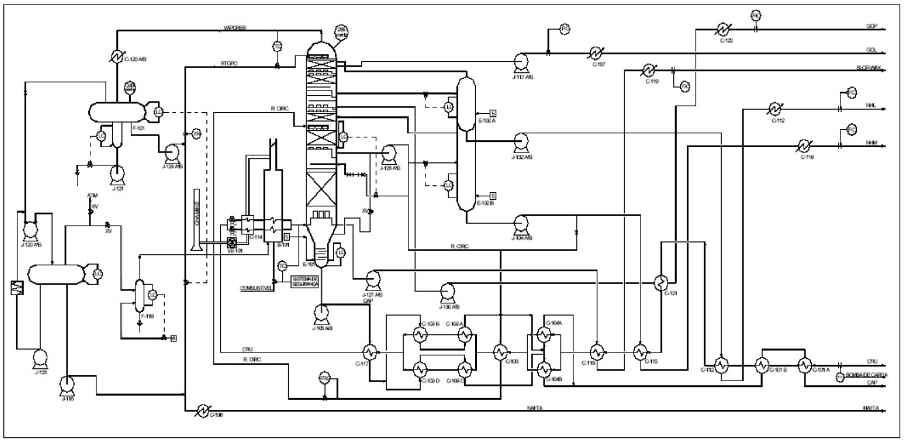

Fig. 1. Subset of a typical flowsheet showing the distillation unit of a chemical plant.

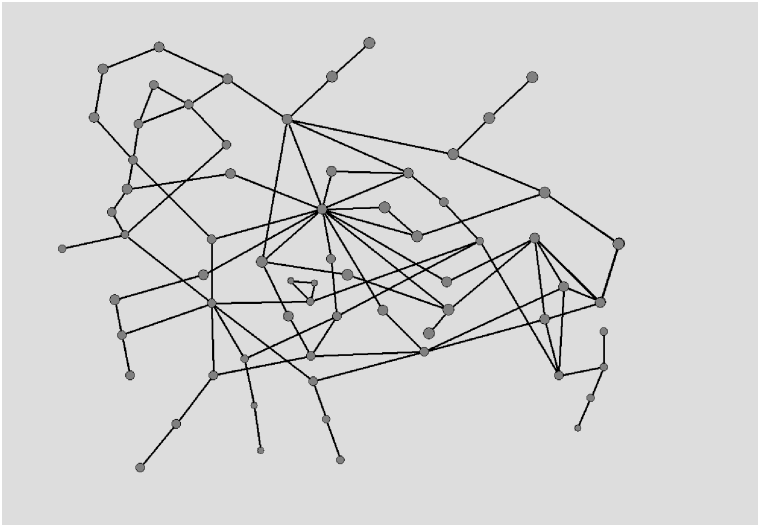

Fig. 2. Complex network representation of Fig. 1. The visualization is obtained by means of the Pajek code for large network analysis (10).

non-determinism represents a crucial step of the design of chemical plants and involves the application of *heuristics* or rules of thumb to undergo the steps in the so-called preliminary process synthesis phase (9). These rules, known to lead to the near-optimal designs in relation to the selection of raw materials, distribution of chemicals, and operations of separation, heat-transfer and pressure-change, have been built from the large *know-how* and experience accumulated during the design of many projects in the past.

In the present study, we show evidence for the existence of a complex topology behind the structure of chemical plants–typified here by oil refineries–that is reminiscent of networks displaying scale-free and hierarchical geometries. Our analysis is based on flowsheets of the distillation and catalytic cracking units that constitute part of two distinct oil refineries, owned and operated by PETROBRAS, the Brazilian State–owned Oil Company. While the first

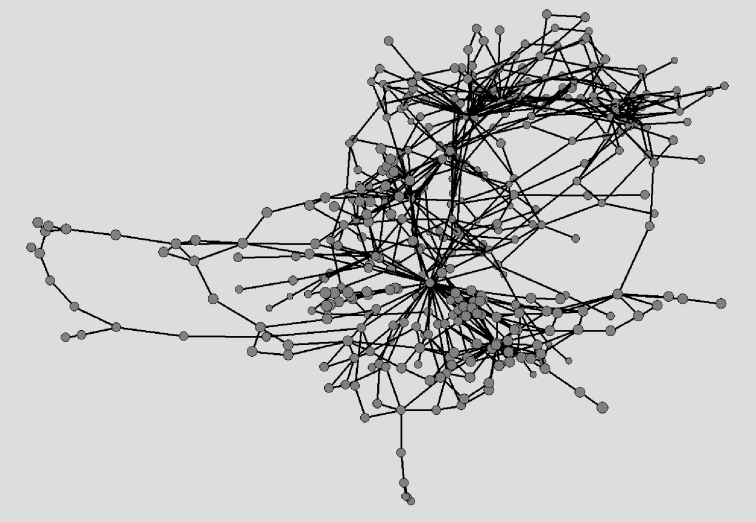

Fig. 3. Pajek visualization (10) of the complex network topology corresponding to the flowsheets of the distillation and catalytic cracking units of Refinery I.

chemical plant, named here Refinery I, can process 8000 m^3/day of exclusively light oil, the second one, or Refinery II, works with a mixture of 80% of heavy and 20% of light oil and has a much larger capacity, of approximately 30000 m^3/day. In Fig. 1 we show the subset of a typical flowsheet comprising some of the basic devices and unitary process elements (e.g., valves, pumps, tanks, heat exchangers, chemical reactors, and distillation columns, among others) connected by a nested flow pipeline. The corresponding network shown in Fig. 2 is simply obtained by associating each of the process units displayed in Fig. 1 to nodes, and their corresponding flow connections to bonds. In Fig. 3, the complex structure of Refinery I is visualized using the Pajek software for large network analysis (10).

The results presented in Fig. 4 provide clear indication that the network topology of Refinery I is scale-free (2). More precisely, its degree distribution for intermediate and large values of the connectivity (degree) k can be properly described as a power-law, $p(k) \sim k^{-\gamma}$, with an exponent $\gamma = 3.3 \pm 0.1$, as calculated from the least-square fit to the data in the scaling region. The degree distribution for Refinery II follows an entirely similar behavior, with an exponent $\gamma = 3.2 \pm 0.2$. The close agreement between these exponents can be substantiated by the fact that the same set of design principles have been applied to the project of both refineries, although their flowsheets are substantially different and purpose-built to perform rather different tasks.

Our calculation for the average length of the shortest path ℓ between two nodes, as defined in Ref. (11), gives $\ell = 5.3$ and 5.9 for Refinery I and II, respectively. When compared with the corresponding sizes N of the refineries, these small values of ℓ suggest, but do not confirm, the presence of a *small-world effect*. Strictly speaking, for a network to be considered *small-world*

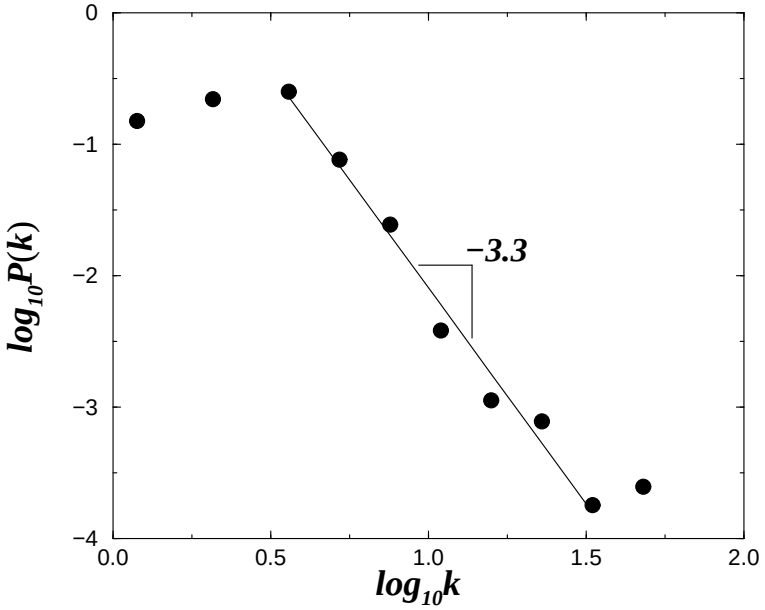

Fig. 4. Log-log plot showing the degree distribution of Refinery I. The solid line corresponds to the best fit to the data in the scaling region of a power-law, $p(k) \sim k^{-\gamma}$, with the exponent $\gamma = 3.3 \pm 0.1$.

	N	$\langle k_i \rangle$	C_{ran}	C	ℓ
Refinery I	452	4.02	0.009	0.21	5.3
Refinery II	470	3.84	0.008	0.16	5.9

Table 1
Sizes and numerical values calculated for complex network parameters of Refineries I and II.

(1; 12; 13), the shortest path ℓ should not only be small, but also grow slower than any positive power of the system size N. Small-world networks also have large clustering coefficient (11). The clustering coefficient for a node i, C_i, is defined as the fraction between the number of connected pairs among its k_i neighbors, n_i, and the number of all possible connections between them,

$$C_i \equiv \frac{2n_i}{k_i(k_i - 1)} \ . \tag{1}$$

Using the definition Eq. (1), we can compute an average cluster coefficient, $C = \langle C_i \rangle$, for the entire network. We find it to be $C = 0.21$ and 0.16 for Refinery I and II, respectively. As shown in Table 1, these values are about 20 times larger than the clustering coefficients computed for random graphs, $C_{\rm ran} = \langle k_i \rangle / N$, with the same average connectivity $\langle k_i \rangle$, thus reinforcing our hypothesis that chemical plants are small-world networks. In order to show the hierarchical aspect of the refinery flowsheets, a more subtle type of analysis

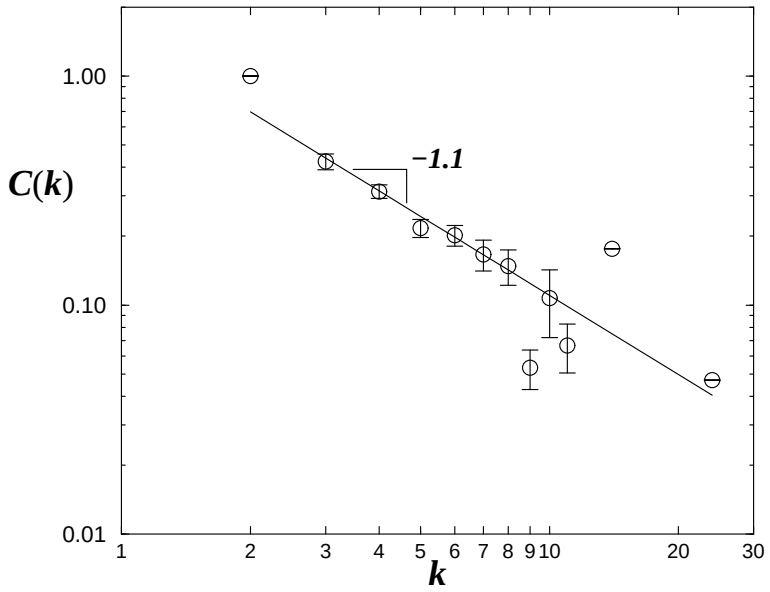

Fig. 5. Logarithmic plot of the clustering coefficient $C(k)$ against the connectivity k for the network topology of Refinery I. The straight line is the least-square fit to the data of a power-law, $C(k) \sim k^{-\beta}$, with the exponent $\beta = 1.1 \pm 0.1$.

is required. Recently, it has been analytically demonstrated that the intrinsic hierarchy of deterministic scale-free networks leads to the scaling relation, $C(k) \sim k^{-1}$, where $C(k)$ represents the average clustering coefficient of nodes with connectivity k. Subsequently, the occurrence of such a behavior has also been used as a way to identify the hierarchical architecture of several real networks (14). Initially, the observation of $C(k)$ versus k including *all nodes* in the data sets of the two refineries revealed fluctuations that were large enough to impair any conclusive description about the hierarchy of both network organizations. However, a detailed analysis of these numerical results indicates the presence of many nodes with $C_i = 0$. These nodes mainly correspond to those constituents of the flowsheets that have very low connectivity k (e.g., valves, pumps, etc.) or are usually added in a secondary stage of the design process to simply provide a single or multiple connection among clusters of more specific unitary processes in the system. As depicted in Fig. 5, the elimination of nodes with $C_i = 0$ from the calculation of $C(k)$ for Refinery I enables us to identify a scaling law, $C(k) \sim k^{-\beta}$ with $\beta = 1.1 \pm 0.1$, that is surprisingly close to the behavior expected for a hierarchical topology. Adopting the same strategy for Refinery II we find an entirely similar result, confirming the validity of our approach.

The identification of several networks with power-law degree distribution in Nature has been generally justified in terms of their evolution through a self-organized process in which hub elements are spontaneously generated and represent the dominant parts of the connected system (13). Here we have shown that man-designed networks composed by unitary processes and de-

vices of a chemical plant can also display scale-free behavior. Moreover, we found significant evidence from real data to suggest that these networks exhibit small-world effect and also have hierarchical organization in their structure (14). Although artificial, we believe that these features stem from the process synthesis schemes tacitly adopted in the design of chemical plants, which involves a combination of *heuristics* and algorithmic techniques (9). We expect these results to be useful in the design stage as well as in the evaluation and characterization of final flowsheets of refinery and other chemical plants.

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