

Process Flow Diagram of an Ammonia Plant as a Complex Network

Zhi-Qiang Jiang, Wei-Xing Zhou, Bing Xu, and Wei-Kang Yuan

State Key Laboratory of Chemical Engineering and Research Center of Systems Engineering,
East China University of Science and Technology, Shanghai 200237, China

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Complex networks have attracted increasing interests in almost all disciplines of natural and social sciences. However, few efforts have been afforded in the field of chemical engineering. An example of complex technological network, investigating the process flow of an ammonia plant (AP) is presented. The AP network is a small-world network with scale-free distribution of degrees. Adopting Newman's maximum modularity algorithm for the detection of communities in complex networks, evident modular structures are identified in the AP network, which stem from the modular sections in chemical plants. In addition, it is found that the resultant AP tree exhibits excellent allometric scaling. © 2007 American Institute of Chemical Engineers *AICHE J*, 53: 423–428, 2007

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Introduction

Complex systems are ubiquitous in natural and social sciences. The behavior of complex system as a whole is usually richer than the sum of its parts, and it is lost if one looks at the constituents separately. Complex systems evolve in a self-adaptive manner and self-organize to form emergent behaviors due to the interactions among the constituents of a complex system at the microscopic level. The study of complexity has been witnessed in almost all disciplines of social and natural sciences (see, for instance, the special issue of *Nature* on this topic in 2001¹). However, engineers seem a little bit indifferent as if engineering is at the edge of the science of complexity. Ottino argues that “engineering should be at the center of these developments, and contribute to the development of new theory and tools”,² and chemical engineering is facing new opportunities.³ The topological aspects of complex systems can be modeled by complex networks, where the constituents are viewed as vertices or nodes, and an edge is drawn between two vertices if their associated constituents interact in certain manners. In recent years, com-

plex networks have attracted extensive interests, covering biological systems, social systems, information systems, and technological systems.^{4–6} Complex networks possess many interesting properties. Most complex networks exhibit small-world traits,⁷ and are scale free where the distributions of degrees have power-law tails.⁸ In addition, many real networks have modular structures or communities.⁹ The fourth intriguing feature of some real networks reported recently is the self-similarity.¹⁰ The studies of complex networks have extensively broadened and deepened our understanding of complex systems.

In the field of chemical engineering, chemical reactions and transports of mass, energy and momentum have been the traditional domains for about five decades, where the topological properties are of less concerns. Amaral and Ottino have considered two examples for which the way constituents of the system are linked determines transport and the dynamics of the system, that is, food webs and cellular networks.¹¹ In this article, we present an example of complex technological network in traditional chemical engineering, studying the topological properties of the process flow of an ammonia plant.

The network studied here is abstracted from the process flow diagram of the Ammonia Plant of Jiujiang Chemical Fertilizer Plant (Jiangxi Province, China). The scale of the plant is 1000MT/D. In the construction of the Ammonia Plant network (AP network), towers, reactors, pumps, heat

Correspondence concerning this article should be addressed to W.-X. Zhou at wxzhou@ecust.edu.cn.

exchangers, and connection points of convergence and bifurcation of pipes are regarded as vertices. Only the equipments and pipes carrying raw materials, byproducts, and products are considered in the construction of network. The utility flows are not included in the network. The pipes connecting the vertices are treated as edges. The AP network constructed has 505 vertices and 759 edges.

AP Network Exhibits Small-World Effect

The average minimum path length is among the most studied quantity in complex networks.⁴⁻⁶ When regarding the AP network as an undirected network, we compute the average minimum path length $\langle l \rangle = 7.76$ with a standard deviation $\sigma_l = 2.65$. We find that the distribution of l is Gaussian. The skewness is 0.17, and the kurtosis excess is 0.01, which is close to the theoretical value 0 of a Gaussian distribution. The average minimum path length, and its fluctuation can also be estimated by a Gaussian fit to the data, which presents $\langle l \rangle = 7.85$, and $\sigma_l = 2.74$.

In most small-world networks, the average minimum path length is somewhat larger than that for a random graph.⁷ It is interesting to compare the average minimum path length of the real ammonia plant network with that of model networks. The null model is the maximally random networks with the same number of nodes and the same degree sequence as the real network. There are several methods for the generation of random graphs with prescribed degree sequences, and the chain switching method gives accurate results with acceptable computational time,¹² which was used in the detection of rich-club structure,¹³ and is the very null model in the statistical tests of network topological properties.¹⁴ Adopting the chain switching method, we have generated 12,400 random networks. The average minimum path length l_{rand} of each model network is calculated. It is found that $l_{\text{rand}} = 5.90 \pm 0.07$. What is striking is that the maximum of l_{rand} is 6.15, much smaller than $\langle l \rangle = 7.76$.

The clustering coefficient C_i of vertex i is a measure of the cluster structure indicating how much the adjacent vertices of the adjacent vertices of i are adjacent vertices of i . Mathematically, C_i is defined by

$$C_i = \frac{E_i}{k_i(k_i - 1)/2} \quad (1)$$

where E_i is the number of edges among the adjacent vertices of i .⁷ The average clustering coefficient $C = \langle C_i \rangle$ is 0.083, which is comparable to other technological networks.⁵ Using the same database of the maximally random networks, we find that $C_{\text{rand}} = 0.0075 \pm 0.0036$, and the maximum clustering coefficient of random networks is 0.025, much smaller than $C = 0.083$ for the ammonia plant network. This is the evidence supporting that the AP network is a small-world network.⁷

AP Network is Scale-Free

The degree k of a vertex of a network is the number of edges connected to the vertex. Degree distributions of vertices are perhaps the most frequently investigated in the literature of complex networks.⁴⁻⁶ The degree distributions of scale-free networks have fat tails following power laws

$$p(k) \sim k^{-(\mu+1)} \quad (2)$$

Several mechanisms of scale-free distributions have been proposed, such as preferential attachment and its variants⁴ and fitness of vertices.^{15,16} In order to estimate the probability distribution of a physical variable empirically, several approaches are available. For a possible power-law distribution with fat tails, cumulative distribution or log-binning technique are usually adopted. A similar concept to the complementary distribution, called rank-ordering statistics,¹⁷ has the advantage of easy implementation, no information loss, and being less noisy.

Consider N observations of variable k sampled from a distribution whose probability density is $p(k)$. Then the complementary distribution is $P(y > k) = \int_k^\infty p(y)dy$. We sort the n observations in nonincreasing order such that $k_1 \geq k_2 \geq \dots \geq k_n$ where n is the rank of the observation. It follows that $NP(k \geq k_n)$ is the expected number of observations larger than or equal to k_n , that is

$$NP(k \geq k_n) = n \quad (3)$$

If the probability density of variable k follows a power law that $p(k) \sim k^{-(\mu+1)}$, then the complementary distribution $P(k) \sim k^{-\mu}$. An intuitive relation between k_n and n follows

$$k_n \sim n^{-1/\mu} \quad (4)$$

A rigorous expression of Eq. 4, by calculating the most probable value of k_n from the probability that the n -th value equals to k_n gives¹⁷

$$k_n \sim \left(\frac{\mu N + 1}{\mu n + 1} \right) \quad (5)$$

When $\mu N \gg 1$ or equivalently $1 \ll n \leq N$, we retrieve Eq. 4. A plot of $\ln k_n$, as a function of $\ln n$ gives a straight line with slope $-1/\mu$ with deviations for the first a few ranks if k is distributed according to a power law of exponent μ . We note that the rank-ordering statistics is nothing but a simple generalization of Zipf's law,¹⁷⁻¹⁹ and has wide applications, such as in linguistics,²⁰ the distribution of large earthquakes,²¹ time-occurrences of extreme floods,²² to list a few. More generally, rank-ordering statistics can be applied to probability distributions other than power laws, such as exponential or stretched exponential distributions,²³ normal or log-normal distributions,¹⁷ and so on.

In Figure 1 is shown the rank-ordering analysis of the in-degree, out-degree and all-degree of the AP network in log-log plot. We see that the AP network is scale-free. Linear regression of $\ln k_n$ against $\ln n$ gives the following exponents: $1/\mu = 0.419 \pm 0.010$ for all-degree, $1/\mu = 0.407 \pm 0.009$ for in-degree, and $1/\mu = 0.4443 \pm 0.008$ for out-degree. Therefore, we have $\mu = 2.39 \pm 0.06$ for all-degree, $\mu = 2.46 \pm 0.05$ for in-degree, and $\mu = 2.31 \pm 0.04$ for out-degree.

Modular Structures in the AP Network

Brief review

In the recent years, much attention has been attracted to the modular clusters or community structures of real networks,

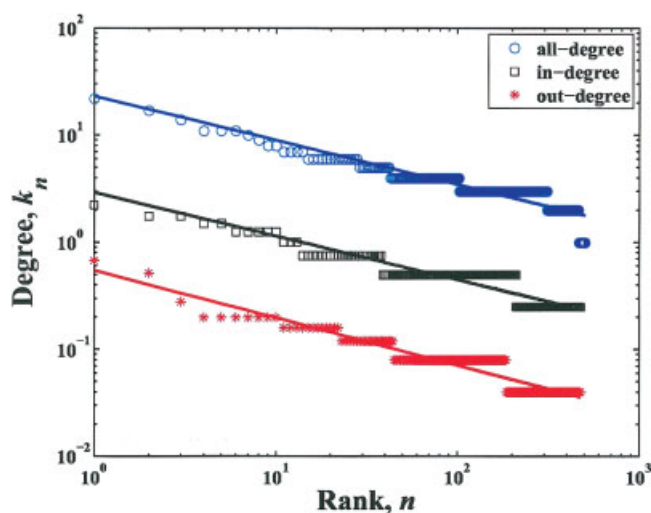


Figure 1. Rank-ordering analysis of the in-degree, out-degree, and all-degree of the AP network.

We have translated vertically the in-degree line by 4 and the out-degree line by 25 for better presentation. The lines are the best fit of tail distribution to Eq. 4. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

such as metabolic networks,^{24,25} food webs,^{26,27} social networks,^{26,28–30} to list a few. There are rigorous definitions for community. A strong community is defined as a subgraph of the network requiring more connections within each community than with the rest of the network, while in a weak community the total number of connections of within-community vertices is larger than the number of connections of the vertices in the community with the rest of the network.^{31,32} However, in most cases in the literature, community is only fuzzily defined in the sense that the connections within communities are denser than between communities.

Different types of algorithms have been developed for the detection of communities.⁹ Sokal and Michener proposed the average-linkage method,³³ which was extended to the hierarchical clustering algorithm later.³⁴ In 1995, Frank developed a method for direct identification of nonoverlapping subgroups,³⁵ which was applied to detect compartments in food webs.²⁷ Girvan and Newman proposed a divisive algorithm that uses edge betweenness centrality to identify the boundaries of communities,^{26,36} which is now widely known as GN algorithm. Based on the concept of network random walking, Zhou used dissimilarity index to delimit the boundaries of communities, which was reported to outperform the algorithm based on the concept of edge betweenness centrality.^{37,38} An alternative divisive algorithm of Radicchi et al. is based on the edge clustering coefficient, related to the number of cycles that include a certain edge.^{31,32} Another well-known algorithm is Newman's maximum modularity algorithm, which is a type of agglomerative algorithm.^{39,40}

Many other algorithms have been presented, for instance, the Kernighan-Lin algorithm,⁴¹ the spectral method which takes into account weights and link orientations and its improvement,^{42,43} the resistor network approach which concerns the voltage drops,⁴⁴ the information centrality algorithm that consists in finding and removing iteratively the edge with the

highest information centrality,⁴⁵ a fast community detection algorithm based on a q -state Potts model,⁴⁶ an aggregation algorithm for finding communities of related genes,⁴⁷ the maximum modularity algorithm incorporated with simulated annealing,²⁵ the agent-based algorithm,⁴⁸ the shell algorithm,⁴⁹ and the algorithm based on random Ising model and maximum flow.⁵⁰

Community structure of the AP network

We apply Newman's maximum modularity algorithm^{39,40} to study the community structure of the AP network. The resultant AP tree is illustrated in Figure 2, which is not in the form of dendrogram. The shapes of the vertices represent different sections of the process flow of the AP: SGP section-oil (solid circles), rectisol section-oil (horizontal ellipses), CO-shift section (vertical ellipses), synthesis and refrigeration section (open circles), air separation section (triangles), nitrogen washing section (vertical diamonds), steam superheater unit (horizontal diamonds), ammonia storage and tank yard (rectangles), and equipments of waste treatment (squares). The maximum value of the modularity is $Q = 0.794$, which is among the largest peak modularity values reported for different networks (if not the largest), and, thus, indicates a very strong community structure in the investigated network.

It has been found that random graphs and scale-free networks have modularity with analytic expressions,⁵¹ which allows us to check if the modularity observed in the AP network is mathematically significant or not. Since the modularity of a scale-free network with $S = 505$ nodes and connectivity $m = 749/505$ is

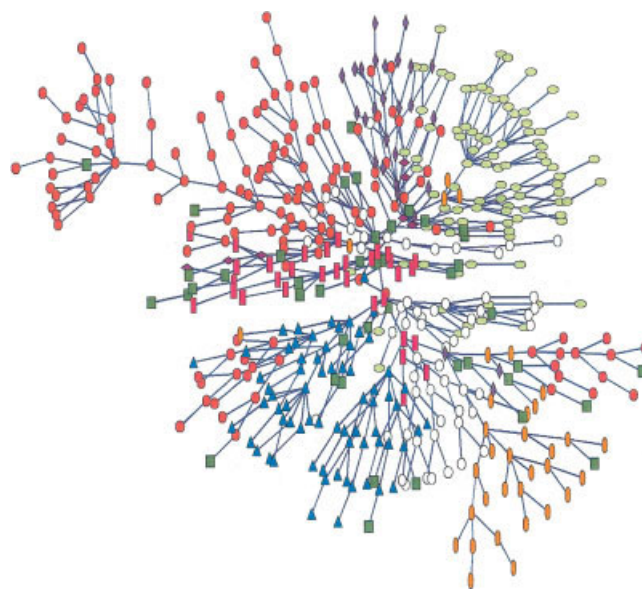


Figure 2. Modular structure of the AP network.

The shapes of the vertices represent different sections of the process flow of the Ammonia Plant. This figure was produced with Pajek.⁵⁹ [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

$$Q_{\text{SF}} = \left(1 - \frac{2}{\sqrt{S}}\right) \left(a + \frac{1-a}{m}\right) = 0.6773 \quad (6)$$

which is again much smaller than $Q = 0.794$, showing that the modularity of the AP network is significant. Note that $a = 0.165$.⁵¹ For an Erdős-Rényi random graph with $S = 505$ nodes and connection probability $p = 749 / (505 \times 504/2) = 0.0059$, the maximal modularity is

$$Q_{\text{ER}} = \left(1 - \frac{2}{\sqrt{S}}\right) \left(1 - \frac{2}{pS}\right)^{2/3} = 0.6995 \quad (7)$$

The fact that Q is greater than Q_{ER} indicates that the modular structure extracted from the AP network could not be attributed to the fluctuation of random graphs and, is, thus, still very significant.

Alternatively, we can use the same null model which employs the chain switching algorithm to generate maximally random networks with the same degree sequence of the AP network. We find that $Q_{\text{rand}} = 0.440 \pm 0.009$, and the maximum of the modularity of model networks is 0.469, which is much smaller than $Q = 0.794$. This test provides further evidence that the modular structure in the AP network is statistically significant.

The modular structures of chemical plant networks do not come out as a surprise. In a chemical plant, raw materials are fed into the process flow network and react from one section to another successively, although there are feedbacks from later sections than between sections. Therefore, a section is naturally a community. In Figure 2, most of the vertices in a given section are recognized to be members of a same community. The vertices of the storage and tank yard (rectangles) are the most dispensed in Figure 2. This is expected since these tanks are linked from and to different sections in the process, which shows the power of Newman's maximum modularity algorithm for community detection.

Allometric scaling of the AP tree

The network shown in Figure 2 is actually a tree. Trees exhibit intriguing intrinsic properties other than nontree networks, among which is the allometric scaling. Allometric scaling laws are ubiquitous in networking systems such as metabolism of organisms and ecosystems river networks, food webs, and so forth.^{52–58} The original model of the allometric scaling on a spanning tree was developed by Banavaret al.⁵⁶ The spanning tree has one root and many branches and leaves, and can be rated as directed from root to leaves. Mathematically, each node of a tree is assigned a number 1 and two values, and are defined for each node in a recursive manner as follows

$$A_i = \sum_j A_j + 1 \quad (8a)$$

and

$$S_i = \sum_j S_j + A_i \quad (8b)$$

where j stands for the nodes linked from i .⁵⁶ In a food web, i is the prey and j 's are its predators (thus, the nutrition flows from i to j 's). The allometric scaling relation is then highlighted by the power law relation between S_i and A_i

$$S \sim A^\eta \quad (9)$$

For spanning trees extracted from transportation networks, the power law exponent η is a measure of transportation efficiency.^{56,58} The smaller is the value of η , the more efficient is the transportation. Any spanning tree can range in principle between two extremes, that is, the chain-like trees and the star-like trees. A chain tree has one root and one leaf with no branching. Let's label leaf vertex by 1, its father by 2, and so forth. The root is labeled by n for a chain-like tree of size n . The recursive relations (Eq. 8) become $S_i = S_{i-1} + A_i$ and $A_i = A_{i-1} + 1$ with termination conditions $A_1 = S_1 = 1$. It is easy to show that $A_i = i$ and $S_i = i(i+1)/2$. Asymptotically, the exponent $\eta = 2^-$ for chain-like trees. For star-like trees of size n , there are one root and $n-1$ leaves directly connected to the root. We have $A = S = 1$ for all the leaves and $A = n$ and $S = 2n-1$ for the root. It follows approximately that $\eta = 1^+$. Therefore, $1 < \eta < 2$ for all spanning trees.

We note that not all trees have such allometric scaling. Consider for instance the classic Cayley with n generations, where the root is the first generation. The A and S values of the vertices of the same generation are identical. If we denote A_i and S_i for the vertices of the $(n+1-i)$ -th generation, the iterative equations are $A_{i+1} = 2A_i + 1$ and $S_{i+1} = 2S_i + A_{i+1}$, resulting in $A_i = 2^i - 1$, and $S_i = (i-1)2^i + 1$. This leads to $S = [\log_2(A+1) - 1]A + \log_2(A+1)$. Obviously, there is no power-law dependence between A and S .

We apply this framework on the AP tree. The calculated S is plotted in Figure 3 as a function of A . A nice power-law relation is observed between S and A . A linear fit of $\ln S$ against $\ln A$ give $\eta = 1.21$ with regression coefficient 0.998. The trivial point ($A = 1$; $S = 1$) is excluded from the fitting.⁵⁸ This value of η is slightly larger than $\eta = 1.13 \sim 1.16$ for food webs,⁵⁸ but much smaller than $\eta = 1.5$ for river networks.⁵⁶ This analysis is relevant when the flux in the pipes and reactors are considered for the investigation of the transportation efficiency, as an analogue to the river network and biological network.^{52,56}

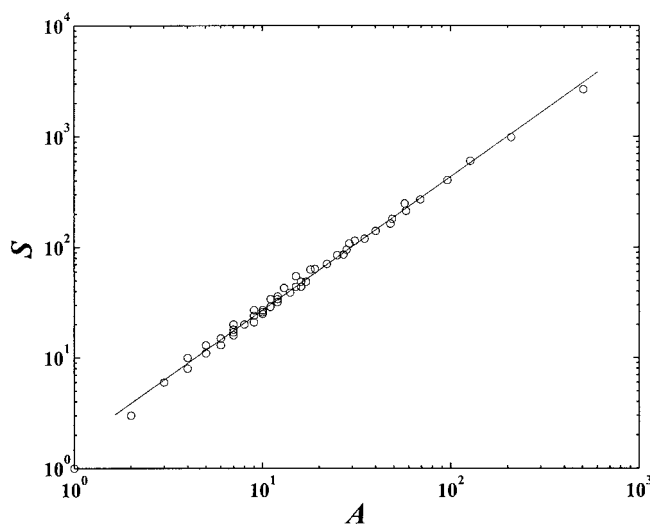


Figure 3. Power-law scaling of S against A . The line represents the power-law fit to the data.

Concluding Remarks

We have studied a complex technological network extracted from the process flow of the Ammonia Plant of Jiujiang Chemical Fertilizer Plant in Jiangxi Province of China. We have shown that the ammonia plant network is a small-world network in the sense that its minimum average path length $\langle l \rangle = 7.76$, and global clustering coefficient $C = 0.083$ are, respectively, larger than their counterparts $l_{\text{rand}} = 5.90 \pm 0.07$ and $C_{\text{rand}} = 0.0075 \pm 0.0036$ of a set of 12,400 maximally random graphs having the same degree sequences of the real AP network. We found that the shortest path lengths between two arbitrary vertices are distributed according to a Gaussian formula. The distribution of degrees follows a power law with its exponent being $\mu = 2.31 \sim 2.46$, indicating that the AP network is scale-free.

We have reviewed briefly diverse existing algorithms for the detection of community structures in complex networks, among which Newman's maximum modularity algorithm is applied to the AP network. The extracted modular structures have a very high-modularity value $Q = 0.794$ signaling the significance of the modules, which is confirmed by statistical tests. These modular structures are well explained by the workshop sections of the ammonia plant. We have constructed a spanning tree based on the community identification procedure and found that the resultant AP tree exhibits excellent allometric scaling with an exponent comparable to the universal scaling exponent of food webs.

In summary, we have studied the topological properties of the AP network from chemical engineering. More sophisticated networks can be constructed from process flows in chemical industry. There are still other open problems even in this small AP network, such as the origin of the scale-free feature, what we can learn from these topological features, robustness and sensitivity analysis on the mass flows to find out bottlenecks in the process or figure out how jamming of the nodes or cascade failure of the system can occur, to list but a few. We hope that this work will attract more affords in this direction. Further researches on complex networks containing information of transports and reactions will unveil useful properties, and benefit the field practically and theoretically.

Acknowledgments

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