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Complex Reaction Networks in High Temperature Hydrocarbon Chemistry Supplementary Information

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1 A Primer on Graph and Network Theory

We abstract almost all the discrete systems by the perception of the units of building-blocks and their relations. This unintentionally natural behavior is origin of development of the networked understanding on those systems. In this sense, all the interconnected systems of the units are networks. Many physical systems which are apparently networked help this view such as The Internet, biological structures e.g. nervous and circulatory systems, electric power distribution grids, highways and roads, crack patterns of solid bodies. However the science of networks traditionally is more about abstract connections for example relationships of people in societies and communities, The World Wide Web, biochemical and chemical reactions, the economy, trade between companies and epidemic disease. In the last decade, a more powerful network theory has been evolved to understand "complex networks" which are extremely large from thousands to billions of units and irregular in their topology and behavior. The complex network theory shows surprising theoretical success by resolving the systems that are nearly impossible to model before. Now, thanks to the network theory, it is known that wide ranging complex systems obey the same laws and highly predictable. This success makes the network theory one of the major mathematical analysis tools of the modern science.

In the next section, we try to illustrate fundamental notions of graph theory to build a background and emphasis the important points in view of our study. For the topics given in the main text we here only discuss complementary details. The definitions are given in the same order of their appearances in the main text. Throughout the next section we benefit from the literature reviews [1, 2, 3, 4, 5] discussing network theory in a great detail. Thanks to popularity of the field there are numerous books, review papers and surveys focused on different aspects of the theory and applications. In order to learn information for broader sense, Barabási's book "Linked: The New Science of Networks [6]" and Newman's book "Networks: An Introduction [7]" are widely accepted introductory textbooks.

1.1 Definitions

Graphs: Graph theory is the mathematics of networks which are topologically equivalent to graphs. In practice, graphs and networks are called interchangeably but we choose to use the "graph" term specifically for mathematical objects while the "network" generically. A graph is simply a graphical representation of vertices (or nodes, points, sites, actors depending on scientific field, singular: vertex) connected by edges (or lines, arcs, links, bonds, ties depending on scientific field). Mathematically this is set G of vertices and edges: G = (V, E). Numbers of vertices $n_V = N$ and edges $n_E = L$ in a graph are called "size" and "order" of the graph, respectively.

Fundamental Graph Types: Graphs can be weighted/unweighted and directed/undirected. If the relations of network units have intensity depending on the relations then the edges of graph have "weight" and it is called weighted graph. In directed graphs (digraphs) edges have strict directions and $E_{i,j} \neq E_{j,i}$ where $E_{i,j}$ is the edge between the vertices of i and j. In reaction networks, mass flux is the weight and for the irreversible reactions edges have directions according to their equilibrium. It is also possible to connect two vertices with multiple edges in "multigraphs". Chemical reactions can be drawn directly as a "hypergraph" in which edges connect any number of vertices arbitrarily. Unfortunately current practical computational techniques in literature are highly limited for hypergraphs and even for the graph types above. Thus "simple graphs" which are unweighted, undirected graphs without loops and multiple edges are widely used in practice since they are computationally very efficient and they have mature and consistent mathematical background.

Next, we demonstrate visual examples of various graph types.

A simple graph with 4 vertices and 5 edges can be drawn straightforwardly:



In the graph below you can find all fundamental graph characteristics with directed and weighted edges as well as loops (w_n is the weight, arrow is the edge direction):



And this is a (directed) hypergraph which is also an excellent representation of chemical reactions:



Adjacency Matrix: Graphs basically are illustrations and cannot be used in calculations. In order to implement mathematical operations, graphs must be represented in various forms for example matrices or lists. Adjacency matrix is the common tool for that goal and given by $N \times N$ $\mathbf{A} = [a_{i,j}]$ square matrix where N is the number vertices and $a_{i,j} = 1$ if there is an edge between i and j vertices otherwise $a_{i,j} = 0$. In the case of weighted graph, if there is an edge then $a_{i,j} \in \mathbb{R}$ and magnitude of $a_{i,j}$ is the weight. In undirected graphs adjacency matrix is symmetric and in simple graphs its diagonal is full of zeros.

Graph Measures (Metrics): Characteristic quantities defining topological and structural properties of a graph. Local measures are defined for individual vertices while global measures are calculated for whole graph.

Degree of a Vertex: The simplest network metric is the degree, k of a vertex which is the total number of the edges connected to that vertex or the number of the nearest neighbors of the vertex. In directed networks vertices have in-degree and out-degree for incoming and outgoing edges. Averaging over the number of vertices gives its global form average degree: $\langle k \rangle = 1/N \sum_{i=1}^{N} k_i$. Statistics of the degree which will be discussed later tells us essence of the graph topology since it is the connection pattern. For example, a vertex with high degree frequently corresponds to the important units for their systems. See Fig. 3 of the main text for the related results.

Graph Density: This is the ratio of the number of the edges to the maximum possible number of the edges (for undirected simple graphs):

$$Density = \frac{L}{\frac{N(N-1)}{2}}$$

In this sense, dense graphs are heavily connected while if a graph is loosely connected then it is "sparse". Mathematically, if $L = O(N^2)$ then graph is dense and if $L \ll (N(N-1))/2$ then graph is sparse (for undirected simple graphs). Note that if L = (N(N-1))/2 it is called "complete graph" (for undirected simple graphs).

Graph Routing: Routes on a graph have species definitions and extremely important applications; a "walk" is a sequence of edges, a "path" is a walk between two specific i and j vertices by crossing each mid-route points only once, "length" of a path is the number of edges on that path, a "cycle" is a path starting and finishing at the same vertex, a "geodesic" or "shortest path" is a path ensuring the minimum walk. "Distance" between two vertices is the number of edges on the shortest path between them and the largest distance of a graph is called the "diameter" of that graph. The "average path length" is the mean of the shortest path lengths between all pairs of vertices:

$$\langle l \rangle = \frac{1}{N(N-1)} \sum_{i \neq j} d_{i,j}$$

where $d_{i,j}$ is the distance between i and j vertices.

Clustering: This class of generic measures quantifies how likely connected i and j vertices could have common (shared) connections to a third vertex. In this context, clustering is also the measure of tendency of graph to form sub-clusters. A subgraph is a vertex set which is subset of the parent graph. Community or cluster is the subset consisting of more densely connected vertices in comparison to other graph segments. Cliques are vertex subsets in the form of complete subgraphs in which all the vertices are connected each other in those subsets. In reaction networks we propose that clusters and cliques might have meanings related to reaction mechanism parts. In the literature of network theory many equation and model is reported to formulate clustering in the form of clustering coefficients. In this study however we choose to discuss widely used transitivity for unipartite graphs and square clustering coefficient for bipartite graphs (see the main text for details).

Assortativity: Assortative mixing is graph theory counterpart of the "like dissolves like" principle of chemistry. In assortative mixing, vertices select the other vertices to connect according to the

similarity of their individual network measures [2]. If same type vertices favor each other more likely this is an assortative network otherwise it is a disassortative network. For example our society (social networks) is mainly based on assortative relationships: people choose to connect other people when they are similar in income level, race or opinion. It is possible to evaluate assortative mixing using any of the graph measures however in scientific literature the prevalent method is to calculate whether the vertices select other vertices to connect by considering their degree (i.e. degree based assortativity). This can be done via the Pearson correlation coefficient of the degrees for the pairs of the connected vertices [8]:

$$r = \frac{1}{\sigma_q^2} \sum_{jk} jk(e_{jk} - q_j q_k)$$

Where e_{jk} is the fraction of edges connecting vertices of the types j and k [9], $q_k = \sum_j e_{jk}$, σ_q is the standard deviation for q. In other words, the numerator is the degree-degree correlation and the denominator is the variance as a normalization factor. This form of the Pearson correlation coefficient is called assortativity coefficient r which is $-1 \leq r \leq 1$ and r > 0 when network is assortative, r < 0 when network is disassortative and r = 0 in the case of no assortative mixing [8]. According to the definition of r, assortative mixing is determined by the similarity of degrees of vertices. In this study we also follow the same method to assess the time-dependent degree assortativity of reaction networks and the results are presented in Fig. 3 of the main text.

Modularity: A "*connected component*" is a subgraph whose all vertices are connected by paths directly or indirectly. A "*module*" is the generalization of this concept and modularity coefficients in the literature determine how subgraphs of same type vertices are well separated. We use modularity coefficient from Clauset et al. [10]:

$$Q = \frac{1}{2L} \sum_{vw} \left[a_{vw} - \frac{k_v k_w}{2L} \right] \delta(c_v, c_w)$$

where L is the number of edges, a_{vw} is the elements of adjacency matrix, k is degree and $\delta(c_v, c_w)$ is a function which is equal to 1 if communities $c_v \equiv c_w$ and 0 otherwise.

Degree Distribution: Degree distribution function P(k) of a graph gives the probability or the fraction of a vertex that its degree is k. Degree distribution is among the most important network statistics since it is easily possible to deduct global topological information. Complex networks usually are classified by their degree distributions. Most of the real-life networks can be fitted to one of the following statistical distributions:

- Power law
- Exponential distribution
- Poisson distribution

Degree distribution function of power law is $P(k) \propto k^{-\gamma}$ where γ is a positive factor. Majority of the real-life networks are believed to obey power law degree distribution with $2 < \gamma < 3$. Exponential distribution function is $P(k) \propto e^{-\tau k}$ with rate parameter τ . Poisson distribution $P(k) \propto z^k/k!$ with a factor z is important but much pedagogical. Combination of power law and exponential distribution, the power law with exponential cut-off is thought to be valid for some special networks and formulated as $P(k) \propto k^{-\alpha} e^{-\beta k}$. In practice, degree distributions are plotted as a cumulative distribution function in log-log axes. For example, the simplest indicator to detect power law distribution is their empirical degree distribution plot which is a negative slope straight line for log-log cumulative visualization. In our own analysis it is found that reaction networks follow the exponential degree distribution (see the main text) as one can detect visually from the line forms of the schematical representation of power law and exponential degree distribution plots given below:



Network Models: Global topologies of real-life and complex networks are observed that they can be modeled using simple mathematical rules. Following network models are traditionally accepted as the foundation of the complex network topologies:

- Erdös-Rényi random graph
- Watts-Strogatz small world model
- Barabási-Albert scale-free networks

One of the simplest but elegant solutions to modeling of graphs was brought by Erdös and Rényi in 1959. In their model, a graph is generated by placing random edges between vertices with a uniform probability. Topological properties of the Erdös-Rényi random graphs can be calculated analytically thanks to its simplicity and in this regard it is also useful for other network models as a template. As anticipated, capabilities of the Erdös-Rényi random graphs are limited in simulation of real life networks since it presumes an equal connection probability for every vertex. Vertices of practical systems are connected by obeying various physical, social, chemical or biological principles. The attempts to find the mathematical models projecting those principles into graphs have become the foundation of modern complex theory. The research of Watts & Strogatz and Barabási & Albert pioneered this research direction in late 1990s. The Watts-Strogatz model constructs a network by starting from a ring graph with specific and constant vertex degree of k and then in each step by shuffling (rewiring) edges with a constant probability of β . This process leads to very distinct "small-world networks" which is one of the major classes of real-life networks. Social scientist Stanley Milgram studied small world phenomenon in 1960s. In Milgram's study, a letter was tried to send by random people to a specific target via only transferring to a direct acquaintance. This social experiment was surprisingly successful yielding the result of that only six people are sufficient ("six degrees of separation") to get the letter to the target. Today it is known that this phenomenon is valid for wide variety of social systems (natural or online). The Barabási-Albert model is one of the most powerful theories to simulate real life networks. According to that model networks are built on the principle of "preferential attachment" i.e. if you are already connected you will have new connections more likely. In the formulation of the Barabási-Albert model one starts with a clique and then adds new vertices by connecting these vertices to existing ones with a probability proportional to the degrees of those existing vertices. What is striking is that this simple model generates considerably realistic two features: power law degree distribution and "scale-free topology". A hierarchic topology with "hub" vertices collecting most of edges in graph is called scale-free which is also extremely tolerant against graph failures like random edges disconnections.

Centrality: Degree centrality of a vertex is simply degree of the vertex. Degree centrality represents the basic idea in the centrality. The vertices with high degree centrality may correspond

to the "sociable" individuals in a society which should be also key people in their environment. Authority and hub centrality is a mutual concept resembling the hierarchical organizations. If the network sends majority of its information traffic to a vertex, this is the authority. Hub vertices control the information traffic between the authority and rest of the network. However in simple graphs authority and hub are always the same vertices. For the definitions of betweenness and closeness centralities please see the main text. Centrality concept is illustrated in the toy example below:



In this graph, vertex f has the highest value for all centrality measures of degree, authority/hub, betweenness and closeness. Note that, for most of the real life networks, centrality measures do not have to overlap at the same vertex and contrary to that example central vertices cannot be discerned by visual examination easily.

2 Method

Chemical reaction mechanisms are computationally simulated using the software package RMG (Reaction Mechanism Generator) which is a rate-based, automated reaction generator [11]. The RMG takes user designated initial conditions (e.g. temperature, pressure, initial composition) and process them using the following tools:

- Numerical solvers of law of mass action ODEs
- Reaction mechanism libraries
- Group additivity estimation of thermodynamic properties
- Master equation solver for pressure dependent reactions

The RMG starts the simulation procedure by reacting initial species in all possible combinations to the reaction families from existing libraries. Integrates the global model in time and determines the significant reactions according to their mass flux. In the second step, the reactions to be selected as significant are reacted to existing species and steps are repeated. This process continues until the main reactant achieves the conversion value specified by user.

We use, for both combustion and pyrolysis, constant temperature and pressure models designated as 2000 K and 1 atm and same kinetic library GRI-Mech 3.0. Mole fractions of initial composition for combustion is Reactant/ O_2 /Ar: 1/1/98 while for pyrolysis is Reactant/Ar: 10/100. 1,3butadiene, acetylene, benzene, ethane, ethylene, methane, methyl isobutyl ketone (MIBK) and toluene are studied as model reactants. RMG is also able to run on time dependent simulations by setting a reaction time which is equivalent of conversion. However we notice tracking of time evolution is difficult since reaction steps actually correspond to very small time intervals. In this regard, in the text we prefer to represent data against conversion and use the terms of conversion and time interchangeably.

After RMG simulations to list full reaction systems for all reactants and conversions we transform each reaction mechanism into a bipartite graph. Considering availability of analysis techniques, we project bipartite CRN graphs into two unipartite graphs of species and reaction. According to the projection rules, these unipartite graphs consist of only species vertices and reaction vertices respectively. Under the fact that species projection has much more information about CRNs, from now on, unless otherwise specified, topological analysis calculations and related network data are only for species graphs. Hence we usually call species graphs and CRNs interchangeably. Topological properties of graphs are then analyzed by R package igraph [9, 12] and Python package NetworkX [13]. In the fitting of empirical degree distribution data by exponential distribution we use the poweRlaw package of R [14]. The fitting procedure of the poweRlaw which relies on the tools of [15] includes the estimation of rate parameter τ and cut-off value k_{min} of Eq. (5) in the main text. Assuming discrete exponential probability distribution, we calculate τ by the maximum-likelihood estimation whilst k_{min} by the minimization of the Kolmogorov-Smirnov statistic.

Analysis of the correlation between percolation threshold and electronic properties of the reactants requires exact numerical value of the thresholds, calculation of the Laplacians of electron distribution and then testing of Pade approximation fitting between them. Percolation threshold is determined as follows: we numerically differentiate conversion - giant component size data, then we calculate pairwise averages of conversions step-by-step, after finding the maximum value of numerical derivative and the corresponding mean conversion, percolation threshold is the conversion value that is the largest one smaller than the pairwise mean conversion of maximum derivative. Remaining percolation analysis requiring giant connected component size, average shortest path length and adjacency matrix largest eigenvalue, is done via igraph for unipartite species projections. In the calculation of electronic properties for reactants using QTAIM, all geometry optimizations were carried with no imposition of symmetry constraints under the hybrid B3LYP functional in conjunction with the 6-31+G(d) basis set; this choice of methodology is a good compromise between computational cost and accuracy for the calculation of properties on sizeable organic molecules. Characterization of the located stationary points as true minima was achieved by analyzing the structure of the diagonalized Hessian matrix in nuclear coordinate space. Energy, frequency and optimization calculations in this work were performed using the Gaussian09 package [16]. Topological properties of the Laplacians of the electron densities were calculated using the AIMStudio suite [17]. Finally, we test our data whether it can be fitted to the Pade approximant which is actually a rational function:

$$R_{d1,d2}^{Pade}(x) = \frac{P_{d1}(x)}{Q_{d2}(x)} = \frac{a_0 + a_1x + a_2x^2 + \dots + a_{d1}x^{d1}}{1 + b_1x + b_2x^2 + \dots + b_{d2}x^{d2}}$$
(1)

We find following equations as the open forms of the Pade approximants fitted to percolation threshold – Laplacian data:

Combustion

$$R_{2,4}^{Pade}(x) = \frac{1.62 \times 10^{-11} - 2.03 \times 10^{-14} x + 6.35 \times 10^{-18} x^2}{1 - 2.43 \times 10^{-3} x + 2.21 \times 10^{-6} x^2 - 8.91 \times 10^{-10} x^3 + 1.35 \times 10^{-13} x^4}$$

Pyrolysis

$$\begin{split} R^{Pade}_{5,7}(x) = \\ \frac{-1.43 \times 10^{-2} + 6.80 \times 10^{-2} x - 1.43 \times 10^{-1} x^2 + 2.68 \times 10^{-4} x^3 - 1.67 \times 10^{-7} x^4 + 3.46 \times 10^{-11} x^5}{1 - 1.51 \times 10^{-1} x + 7.43 \times 10^{-7} x^2 + 4.79 \times 10^{-4} x^3 + 1.93 \times 10^{-1} x^4 - 3.59 \times 10^{-4} x^5 + 2.23 \times 10^{-7} x^6 - 4.61 \times 10^{-11} x^7} \end{split}$$

3 Support to Figures

This section shows accompanying figures for the main text.

(a) 1,3-Butadiene (Combustion)

(b) 1,3-Butadiene (Pyrolysis)



Figure S1. Log-log plot of the complementary cumulative distribution function (CCDF) of the vertex degree distribution for species graphs of combustion and pyrolysis reactions along with their power-law analysis. Filled blue circles are the empirical degree distributions and vertical dashed lines are the average degrees. All of them are shown with an increasing opacity order of the line color from the conversion of 0.2 to 0.99 in the interval of 0.2. Dash-point black curves are theoretical fit by the exponential degree distribution model to the final network (of the conversion 0.99). The insets are the time evolution of Vuong's Test results. For details see the main text.

(g) Ethylene (Combustion)

(h) Ethylene (Pyrolysis)



Figure S1. Continued.



Figure S2. Time dependent change of authority & hub, betweenness and closeness centralities for combustion and pyrolysis mechanisms of a) 1,3-butadiene, b) acetylene, c) benzene, d) ethane, e) ethylene, f) MIBK and g) toluene. Labels in each circle correspond to the species with maximum centrality. Circle size is proportional to magnitude of the maximum centrality but not scaled. Since our networks are undirected, authority and hub centralities are exactly same and shown together. The species with asterisk symbol are radicals. SPC_(#) accounts for the uncertain isomers and long species names each of whose InChI codes are given below:

- $SPC_{(149)}$: InChI=1/C6H5O/c7-6-4-2-1-3-5-6/h1-4,7H
- $SPC_{(282)}$: InChI=1/C6H6/c1-3-5-6-4-2/h3,6H,1-2H2/mult3
- SPC₍₂₈₅₎: InChI=1/C6H6/c1-3-5-6-4-2/h3,5H,1-2H2/mult3
- SPC₍₂₉₈₎: InChI=1/C6H6/c1-3-5-6-4-2/h3,5H,1-2H2/mult3
- SPC₍₃₄₉₎: InChI=1/C2H3O/c1-2-3/h1H3
- SPC₍₈₈₁₎: InChI=1/C3H4O/c1-2-3-4/h1-2H2/mult3
- $SPC_{(3981)}: InChI = 1/C15H14/c1-2-13-9-6-10-15(11-13)12-14-7-4-3-5-8-14/h2-12H, 1H3/mult3.$





Figure S2. Continued.



Figure S3. The Transition State Theory test calculations for three major reaction steps in our mechanisms. The minima of all curves corresponding to stable structures (reactants in our cases) appear to the left of the plot, the high energy points to the right correspond to the products. A common case for radical reactions in chemistry is that if they proceed in one step, then they proceed without a transition state, and this is clearly the case here, therefore, we can not calculate reaction rates using TST.

(a) 1,3-Butadiene



(b) Acetylene



(c) Benzene



Figure S4. The molecular structures for 1,3-butadiene, acetylene and benzene. The structures only include the Laplacians of the electron densities and their local maxima (yellow spheres) not corresponding to atom positions; the global maxima, of course, are located at the carbon atoms. The yellow spheres are the (3,+3) critical points and the surfaces are the Laplacians of the electron densities.



(e) Ethylene



(f) MIBK



 ${\bf Figure ~S4.} {\rm ~Continued.} {\rm ~The~molecular~structures~for~ethane,~ethylene~and~MIBK.}$



Figure S4. Continued. The molecular structure for toluene.

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