Scaling down the reaction system for low-temperature plasma chemistry

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Abstract: Multidimensional simulations with extensive chemical reaction set are computationally intensive, so the scale of reaction set should be properly examined. We propose a graph theoretical approach for scaling down the reaction system of complex plasma-activeted liquid checmitry. We reduced the number of reaction processes by half while maintaining inherent chemical network structure.

Keywords: Low-temperature plasma chemistry, graph theory, network analysis.

1. Introduction

Low-temperature plasmas have attracted attention in various fields such as biology and medicine. The plasma reaction systems, however, tend to become more complex as the number of chemical reaction equations to be considered increases, which can affect the numerical calculation of plasmas. To solve this problem, it has been attempted to scale down the plasma reaction networks using graph theory. Here, scaling down means reducing the number of chemical reaction equations, and the chemical reaction equations are reduced based on the analysis of the plasma reaction networks using graph theory. By using the remaining chemical reaction equations for numerical calculations, it is expected to reduce the calculation time while maintaining the accuracy of the network[1,2].

We previously scaled down focusing on chemical species[2], but now we have attempted to scale down focusing on chemical reaction equations. In this abstract, using a complex liquid-phase chemical reaction network as an example, we propose a method for scaling down the reaction network using graph theory while maintaining the network structure.

2. Methods

2.1. Network of chemical reaction equation

Fig. 1 shows a conceptual network using the chemical reaction equation $OH+OH^- \rightarrow O^- + H_2O$ as an example. Here, OH, OH^-, O^- and H_2O are called nodes, and edges can be drawn between OH and OH^-, O^- and H_2O respectively. In this case, we can create a reactant network(a network connecting reactants) and a product network(a network connecting products) respectively. Also, each edge of the reactant network has the reaction coefficient of the chemical reaction equation containing that edge as its weight.

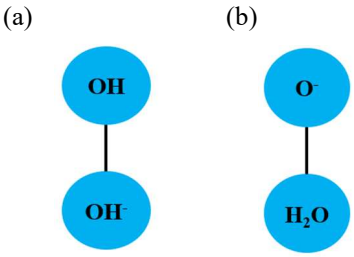

Fig. 1. A conceptual network of the chemical reaction equation through $OH+OH^- \rightarrow O^- + H_2O$.
(a) Reactant network, (b) Product network

2.2. Indexes in graph theory

2.2.1. Degree centrality

Degree is the number of edges that each node has, and degree centrality is the idea that a node with a very high degree is the center of the network[3].

2.2.2. Betweenness centrality and edge betweenness

Betweenness centrality is the degree of bridging or control between nodes[3]. The betweenness centrality of each node is written as:

$$b_i = \sum_{\substack{j>j' \\ (j,j' \neq i)}} \frac{\sigma(j|i|j')}{\sigma(j|j')} = \sum_{\substack{j>j' \\ (j,j' \neq i)}} \frac{\sigma(j|i|j')}{\frac{(N-1)(N-2)}{2}} \quad (1)$$

Then, $\sigma(j|j')$ is the number of shortest paths connecting nodes j and j', N is the total number of nodes, and $\sigma(j|i|j')$ is the number of shortest paths connecting nodes j and j' that pass through node i. From this formula, the betweenness centrality of each node is considered as the number of times the shortest path connecting all node pairs in the network passes through that node. Therefore, if a node is on many shortest paths, its betweenness centrality will be higher, and thus the betweenness centrality of nodes with higher degrees tends to be higher[4].

We can also assume that $\sigma(j|i|j')$ is the number of shortest paths connecting nodes j and j' that pass through edge i, in which case b_i is called edge betweenness. This indicates which edges are most prevalent between nodes in the network[4,5].

2.3. Method of scaling down a reaction system

The method we propose for scaling down a reaction system is stated as:

1. Create reactant and product networks
2. Calculate edge betweenness in the reactant network
3. Remove edges with low edge betweenness

In this abstract, half of the reaction equations that contain edges with low edge betweenness are removed in order to halve the number of chemical reaction equations after scaling down.

3. Results and discussion

3.1. Liquid-phase reactant network diagram

Fig. 2 is reactant network diagrams in the liquid-phase reaction system considering degree centrality before and after scaling down. The chemical species with higher degrees have larger node sizes and are located in the center of the network. Also, the edge with a high reaction coefficient is thicker, so the chemical species with thicker edges in the network indicate that they tend to react together chemically.

These figures suggest that chemical species located near the center of the network, such as OH, O_2, H and O_2^-, react topologically with many chemical species. Then, some chemical species, such as H^+ and O_3, are found to have relatively low degrees but tend to react chemically.

3.2. The change of the reaction set by scaling down

Table 1 is the reaction set of the liquid-phase reactant network before and after scaling down. The number of chemical reaction equations decreased by 50[%], and the number of edges and chemical species decreased by 44[%] and 3[%], respectively. Thus, we could scale down without losing a much number of chemical species.

3.3. The change of index values by scaling down

Fig. 3 is a normalized graph of degree and betweenness centrality in the liquid-phase reactant network before and after scaling down. From this graph, a similar distribution between degree and betweenness centrality could be found even before and after scaling down. This indicates that the scales of the reaction systems change, but the structure of the reaction systems are similar.

4. Conclusion

Using a liquid-phase reaction system as an example, we proposed a method of scaling down focusing on chemical reaction equations. Here, we could reduce the number of chemical reaction equations by half while maintaining the network structure. We believe that this method of scaling down can be used for plasma reaction systems which are as complex networks as liquid-phase reaction systems.

5. Acknowledgements

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6. References

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(a) (b)

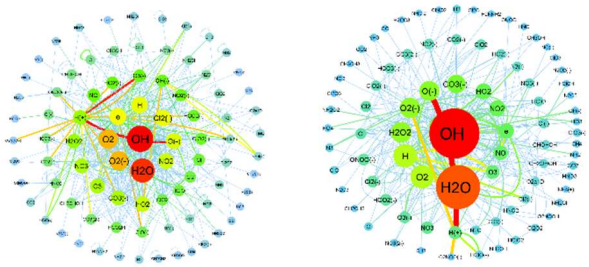

Fig. 2. Reactant network diagrams in the liquid-phase reaction system. (a) Before scaling down, (b) After scaling down

Table 1. The reaction set of the liquid-phase reactant network before and after scaling down.

	Before scaling down	After scaling down
Species	86	83
Reactions	401	200
Edges	490	272

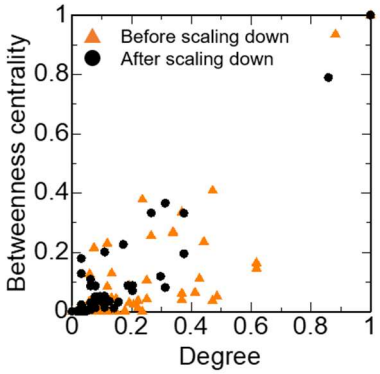

Fig. 3. Normalized graph of degree and betweenness centrality in the liquid-phase reactant network before and after scaling.