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Cascading Propagation Path of Vinyl Chloride Process Risk Based on Complex Network

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Abstract: In the production of vinyl chloride, small parameter fluctuations may lead to large-scale cascade fluctuations, causing serious economic losses and casualties, in order to ensure the safety and stability of production, it is necessary to study the cascade fluctuation propagation path of vinyl chloride production process. In this paper, a complex network model of vinyl chloride production process is constructed based on complex network theory, and the concept of comprehensive degree considering network direction is introduced to identify important nodes in the network: secondly, the fluctuation overload propagation probability and material hazard degree of the edge are used to define the fluctuation overload propagation intensity of the edge; finally, according to the fluctuation overload propagation intensity, the risk propagation path of cascading fluctuations under different overload modes is obtained by using ant colony algorithm, it provides a basis for the prevention of cascade overload and the selection and protection of key monitoring nodes.

Keywords: Cascade fluctuation, Complex network, Fluctuation risk propagation path, Vinyl chloride production.

1. Introduction

Vinyl chloride is an important raw material in the plastic industry. It can also be used as an extractant for dyes and spices. The production process of vinyl chloride is a typical process industrial production with continuity. At the same time, the production process system is huge, and various parts in the production process are interrelated. The fluctuation of one parameter may cause the fluctuation of other parameters in the follow-up, which may lead to the occurrence of cascade failure, and eventually lead to the interruption of production and even vinyl chloride leakage.

At present, scholars' research on cascaded volatility mainly focuses on the establishment of cascaded volatility models [1], the study of resilience in the face of volatility [2], the study of risk propagation paths [3], the study of cascaded volatility mechanisms [4]. It has been widely studied in different disciplines, such as transportation network [5], power network [6], communication network [7], water supply network [8], biological network [9], chemical network [10], which shows that complex network is an effective method suitable for the study of risk cascade propagation path of process parameter fluctuation. Wang and others [10] constructed three cascaded volatility models based on complex network theory, which provided a reference for the model establishment in this paper. But it does not judge the importance of a node from the global view of the network. Based on this, some scholars [11] proposed a method to identify the key nodes of complex networks by considering the various topological characteristics of nodes and the characteristics of the networks they study, but it does not take into account the directionality of complex networks. In this paper, the ant colony algorithm [12] is used to comprehensively consider the topological characteristics of the network and the risk of materials on the basis of other scholars [13] to identify the cascading risk propagation path of parameter fluctuations in the vinyl chloride production process, which provides a certain basis for the prevention of cascading overload and the selection and protection of key monitoring nodes.

2. Methods

2.1. Establishment of Complex Network Model

In the chemical production process, according to the complex network theory, the flow rate of materials in and out of the vinyl chloride production process and the various reaction parameters are abstracted as the nodes of the network, and the interaction relationship between them is abstracted as the edge of the network, defining the adjacency matrix A:

$$A=\begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} \tag{1}$$

where a_{ij} represents whether there is an association between node i and node j.

$$a_{ij}=\begin{cases} 1\text{，node i and node j are related；} \\ 0\text{，node i and node j are not related} \end{cases} \tag{2}$$

The complex network model can be obtained by entering the established adjacency matrix into the software Ucinet6.0.

2.2. Establishment of Cascade Wave Model for Complex Networks

The initial load, load capacity, load redistribution rules for the nodes in this article are as follows.

(1) The initial load of the node: According to the degree of the node and the degree of the neighbor node, the initial load N_i of the node i is defined:

$$N_i=k_i(1+\sum_{m\in\tau_i} k_m)-k_i \tag{3}$$

Where k_i is the degree of node i and τ_i is the set of neighbor nodes of the node.

(2) Load capacity of the node: Assuming that the load

capacity of the node and the initial load are linearly related, the load capacity C_i of the node is defined:

$$C_i=（1+\beta）N_i \tag{4}$$

where B is the tolerance parameter, taking 0.06

(3) Node Load Redistribution Rule: Assuming that node i fails, the load of node i will be assigned to the node to which it points, and if node j is a pointing node of the node i, the load ΔN_j assigned to node j is defined:

$$\Delta N_j=\frac{N_i N_j}{\sum_{m\in\varepsilon_i} N_m} \tag{5}$$

where ε_i is the set of neighbor nodes to which node i points.

2.3. Node importance judgment

Based on the K-shell method, this paper introduces the concept of comprehensive degree. The degree of integration of a node is defined:

$$C(i)=K(i)+\mu_i D(i) \tag{6}$$

where *K(i)* is the degree of the node, *D(i)* is the number of secondary neighbors of the node, and μ_i is the influence coefficient.

According to the degree *K(i)* of the node and the total number *N(i)* of nodes in the two-step neighborhood of the node, μ_i is defined:

$$\mu_i=\frac{K(i)}{N(i)} \tag{7}$$

The mean value of the node's in-degree synthesis $C_{in}(i)$ and out-degree synthesis $C_{out}(i)$ is taken as the final synthesis value:

$$C_{ave}(i)=\frac{C_{in}(i)+C_{out}(i)}{2} \tag{8}$$

2.4. Complex network fluctuation cascade propagation intensity I_{ij}

In a complex network, the stronger the fluctuation propagation ability of an edge, the easier it is for the fluctuation to propagate along this edge. At the same time, a large number of raw materials and products in the production process of vinyl chloride have certain risks, which will also have a certain impact on the cascade propagation of fluctuations. Therefore, the article defines the intensity of fluctuation propagation I_{ij} on the opposite side:

$$I_{ij}=\frac{L_{ij}}{MaxL_{ij}}+\frac{W_{ij}}{MaxW_{ij}} \tag{9}$$

L_{ij} is the fluctuation propagation probability of the edge on the network, which is determined by the fluctuation propagation probability Q_i of the node and the fluctuation propagation capability S_{ij} of the edge. The fluctuation propagation probability Q_i of the node is determined by the fluctuation probability P_i of the node and the propagation capability S_i after the node fluctuates. The fluctuation propagation capability S_{ij} of the edge is determined by the fluctuation propagation capability S_i of the nodes at both ends of the edge. W_{ij} is the risk of materials on the network, including toxic, corrosive and flammable and explosive, taking into account subjective and objective factors, the combination of hierarchical analysis and rough set theory to quantify the risk of materials. Finally, the fluctuation propagation intensity I_{ij} of the edge is obtained.

3. Establishment of Cascade Fluctuation Model for Vinyl Chloride Production Process

3.1. Establishment of Complex Network of Vinyl Chloride Production Process

The process for the production of vinyl chloride by the equilibrium oxychlorination method is shown in Figure 1 and consists of five main parts: chlorination of ethylene, oxychlorination, dichloroethane refining, dichloroethane cracking, vinyl chloride refining.

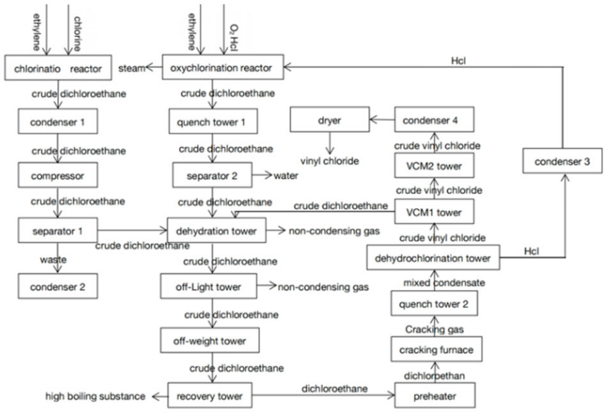


Figure 1. Flow Chart of Production of Vinyl Chloride by Equilibrium Oxygen-chlorine Process

According to the complex network theory, the material flow rate and each reaction parameter in the vinyl chloride production process are abstracted as the nodes of the network, as shown in Table 1.

The adjacency matrix is entered into Ucine6.0 to generate a complex network model as shown in Figure 2.

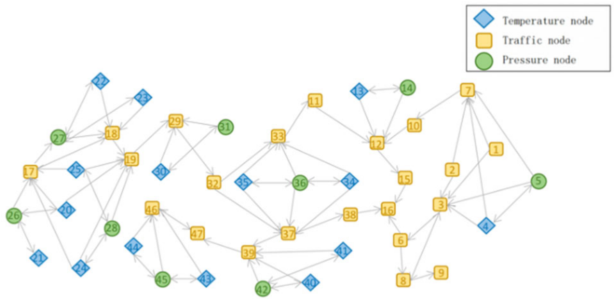


Figure 2. Complex network model of vinyl chloride production process

Table 1. Network Node Definition

No.	Name	No.	Name
1	Flow of chlorine into chlorination reactor	**25**	Bottom temperature of deweight tower
2	Flow of ethylene into chlorination reactor	**26**	Dehydration tower pressure
3	Flow of mixture out of chlorination reactor	**27**	Off-light tower pressure
4	Temperature of chlorination reactor	**28**	Heavy tower pressure
5	Pressure of chlorination reactor	**29**	Flow rate of cracking gas out of cracking furnace
6	Flow of crude dichloroethane out of condenser 1	**30**	Cracking temperature
7	Flow of ethylene tail gas in chlorination reaction	**31**	Cracking pressure
8	Flow of crude dichloroethane into separator 1	**32**	Flow rate of mixed condensate out of quench tower 2
9	Flow of crude dichloroethane out of separator 1	**33**	Flow rate of Hcl out of Hcl tower
10	Flow of ethylene into oxychlorination reactor	**34**	Top temperature of Hcl tower
11	O2 and Hcl flow into the chlorination reactor	**35**	Bottom temperature of Hcl removal tower
12	Flow of crude dichloroethane out of the oxychlorination reactor	**36**	Pressure of Hcl removal tower
13	Temperature of the oxychlorination reaction fluidized bed	**37**	Crude vinyl chloride flow out of Hcl removal tower
14	Pressure of the oxychlorination reaction fluidized bed	**38**	Crude dichloroethane flow out of VCM1 tower
15	Flow of crude dichloroethane out of the quench tower 1	**39**	Crude vinyl chloride flow out of VCM1 tower
16	Flow of crude dichloroethane into the dehydrating tower	**40**	Top temperature of VCM1 tower
17	Flow of crude dichloroethane out of the dehydrating tower	**41**	Bottom temperature of VCM1 tower
18	Flow of crude dichloroethane out of the off-light tower	**42**	Top temperature of VCM1 tower
19	Flow of crude dichloroethane out of the off-weight tower	**43**	Bottom temperature of VCM2 tower
20	Dehydration tower top temperature	**44**	Bottom temperature of VCM2 tower
21	Dehydration tower bottom temperature	**45**	Pressure of VCM2 tower
22	Top temperature of off-light tower	**46**	Crude vinyl chloride flow out of VCM2 tower
23	Bottom temperature of off-light tower	**47**	Vinyl chloride flow out of the dryer
24	Top temperature of deweight tower		

3.2. Vinyl chloride production process Complex network Node importance

First, the Ks value of each node of the complex network model of the vinyl chloride production process is calculated, and then the comprehensive degree of the node is obtained according to the formula (6)-(9), and the results are shown in Figure 3.

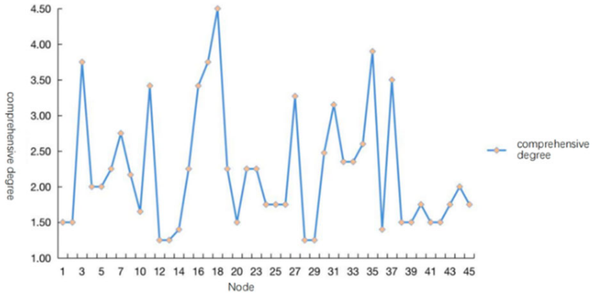
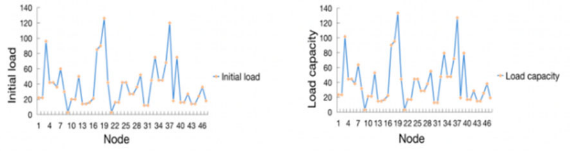


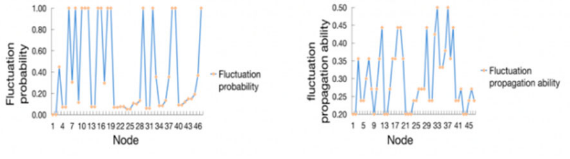
Figure 3. Comprehensive degree of nodes

3.3. VCM production process complex network parameter fluctuation cascade propagation intensity I_{ij}

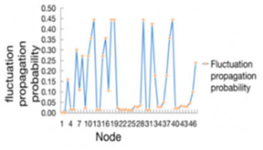
First, according to the formula (3), (4) to find the initial load and load capacity of the complex network node of the vinyl chloride production process, on this basis to obtain the parameter fluctuation probability P_i of the node, the parameter fluctuation propagation capacity S_i of the node and the fluctuation propagation probability Q_i of the node, as shown in Figure 4. The edge's parameter fluctuation propagation capability S_{ij} is then multiplied by the node's parameter fluctuation propagation probability Q_i to obtain the edge's parameter fluctuation propagation probability L_{ij}, as shown in Table 2.



（a）Initial load of the node （b）Load capacity of the node



（c）Volatility Probability （d）Fluctuation propagation capability



（e）Volatility Propagation Probability

Figure 4. Node and edge metrics

Table 2. Fluctuation Propagation Capability S_{ij} of an Edge and Fluctuation Propagation Probability L_{ij} of an Edge

Edge (i→j)	S_{ij}	L_{ij}	Edge (i→j)	S_{ij}	L_{ij}	Edge (i→j)	S_{ij}	L_{ij}	Edge (i→j)	S_{ij}	L_{ij}	Edge (i→j)	S_{ij}	L_{ij}
1→3	0.280	0	**11→12**	0.400	0.144	**24→17**	0.300	0. 003	**31→30**	0.240	0.002	**40→39**	0.340	0.007
1→7	0.280	0	**12→15**	0.355	0.156	**24→19**	0.340	0.003	**32→33**	0.460	0.193	**40→42**	0.255	0.005
2→3	0.280	0	**13→12**	0.320	0.003	**24→28**	0.255	0.003	**32→37**	0.460	0.193	**41→39**	0.340	0.007
2→7	0.280	0	**13→14**	0.200	0.002	**25→17**	0.300	0. 003	**33→11**	0.430	0.077	**41→42**	0.255	0.005
3→6	0.330	0.053	**14→12**	0.320	0.003	**25→19**	0.340	0.003	**34→33**	0.415	0.012	**42→39**	0.355	0.011
3→8	0.315	0.050	**14→13**	0.200	0.002	**25→28**	0.255	0.003	**34→36**	0.355	0.011	**42→40**	0.255	0.008
4→3	0.300	0.006	**15→16**	0.315	0.085	**26→17**	0.315	0.009	**34→37**	0.415	0.012	**42→41**	0.255	0.008
4→5	0.240	0.048	**17→18**	0.400	0.044	**26→20**	0.315	0.009	**35→33**	0.415	0.012	**43→45**	0.220	0.007
4→7	0.300	0.006	**18→19**	0.440	0.194	**26→21**	0.235	0.007	**35→36**	0.355	0.011	**43→46**	0.235	0.007
5→3	0.300	0.006	**19→29**	0.440	0.194	**27→22**	0.315	0.009	**35→37**	0.415	0.012	**44→45**	0.220	0.007
5→4	0.240	0.048	**20→17**	0.360	0.007	**27→23**	0.315	0.009	**36→33**	0.440	0.022	**44→46**	0.235	0.007
5→7	0.300	0.006	**20→19**	0.400	0.008	**28→19**	0.355	0.014	**36→34**	0.355	0.018	**45→43**	0.220	0.011
6→8	0.285	0.086	**20→26**	0.315	0.006	**28→24**	0.255	0.010	**36→35**	0.355	0.018	**45→44**	0.220	0.011
6→16	0.330	0.099	**21→26**	0.235	0.002	**28→25**	0.255	0.010	**36→37**	0.440	0.022	**45→46**	0.255	0.013
7→10	0.300	0.033	**22→18**	0.320	0.006	**29→32**	0.430	0.189	**37→38**	0.430	0.077	**46→47**	0.250	0.025
8→3	0.300	0.081	**22→27**	0.235	0.005	**30→29**	0.340	0.003	**37→39**	0.470	0.085			
8→9	0.235	0.063	**23→18**	0.320	0.006	**30→31**	0.240	0.002	**38→16**	0.360	0.130			
10→12	0.355	0.096	**23→27**	0.235	0.005	**31→29**	0.340	0.003	**39→47**	0.340	0.150			

For the measurement of material hazard W_{ij}, the subjective weight ω_i=(0.27,0.12,0.61) of toxicity, corrosiveness and easy explosion can be obtained, and the calculated weight is reasonable after inspection.The objective weight of explosiveness Z_i=(0.5,0.25,0.25). Finally, the comprehensive weight θ_i=(0.385,0.185,0.43) is obtained. As shown in Table 3, the fluctuation propagation intensity I_{ij} is shown in Figure 5.

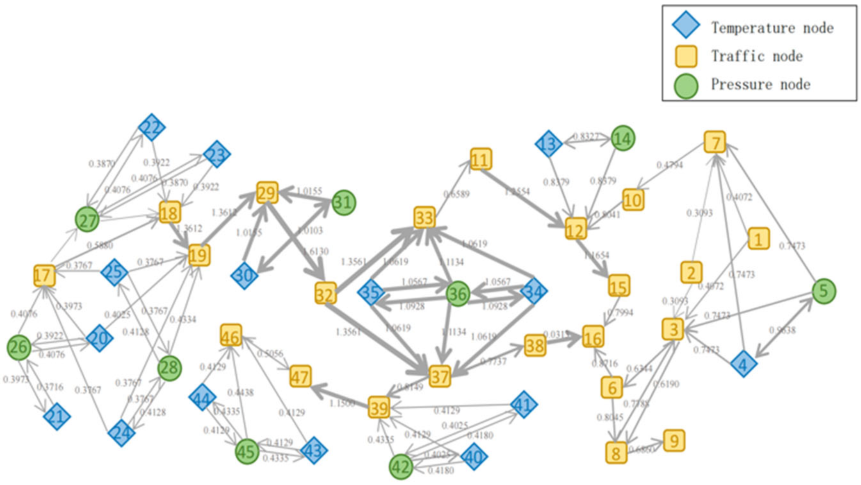


Figure 5. Intensity of wave propagation I_{ij}

Table 3. Hazard degree of materials W_{ij}

Edge (i→j)	W_{ij}	Edge (i→j)	W_{ij}	Edge (i→j)	W_{ij}	Edge (i→j)	W_{ij}	Edge (i→j)	W_{ij}
1→3	3.015	**11→12**	3.800	**24→17**	2.675	**31→30**	7.405	**40→39**	2.790
1→7	3.015	**12→15**	2.675	**24→19**	2.675	**32→33**	2.675	**40→42**	2.790
2→3	2.290	**13→12**	6.090	**24→28**	2.675	**32→37**	2.675	**41→39**	2.790
2→7	2.290	**13→14**	6.090	**25→17**	2.675	**33→11**	1.940	**41→42**	2.790
3→6	2.675	**14→12**	6.090	**25→19**	2.675	**34→33**	7.405	**42→39**	2.790
3→8	2.675	**14→13**	6.090	**25→28**	2.675	**34→36**	7.405	**42→40**	2.790
4→3	5.305	**15→16**	2.675	**26→17**	2.675	**34→37**	7.405	**42→41**	2.790
4→5	5.305	**17→18**	2.675	**26→20**	2.675	**35→33**	7.405	**43→45**	2.790
4→7	5.305	**18→19**	2.675	**26→21**	2.675	**35→36**	7.405	**43→46**	2.790
5→3	5.305	**19→29**	2.675	**27→22**	2.675	**35→37**	7.405	**44→45**	2.790
5→4	5.305	**20→17**	2.675	**27→23**	2.675	**36→33**	7.405	**44→46**	2.790
5→7	5.305	**20→19**	2.675	**28→19**	2.675	**36→34**	7.405	**45→43**	2.790
6→8	2.675	**20→26**	2.675	**28→24**	2.675	**36→35**	7.405	**45→44**	2.790
6→16	2.675	**21→26**	2.675	**28→25**	2.675	**36→37**	7.405	**45→46**	2.790
7→10	2.290	**22→18**	2.675	**29→32**	4.730	**37→38**	2.790	**46→47**	2.790
8→3	2.675	**22→27**	2.675	**30→29**	7.405	**37→39**	2.790		
8→9	2.675	**23→18**	2.675	**30→31**	7.405	**38→16**	2.675		
10→12	2.290	**23→27**	2.675	**31→29**	7.405	**39→47**	2.790		

4. Identification and Analysis of Risk Propagation Path of Cascade Fluctuation in Vinyl Chloride Production Process

Using the ant colony algorithm to solve the cascade fluctuation risk propagation path of the complex network of vinyl chloride production process when the three fluctuation modes of important node fluctuation, high load node fluctuation and random fluctuation are 10%, 20% and 30%, respectively, the fluctuation propagation path is shown in Figure 6.

It can be seen from fig. 6 that when the load capacity is 100 and there are 10% important node fluctuations, the cascade fluctuation risk propagation path of vinyl chloride production process is 35 → 36 → 34 → 37 → 39 → 47, which indicates that in the initial production process, when a few nodes fluctuate, nodes 35, 36, 34, 37, 39 and 47 are more prone to cascade fluctuations, it can be seen that the reaction conditions in the Hcl removal tower are the most severe, and the flow rates of materials out of the Hcl removal tower, the VCM1 tower and the dryer also need to be controlled more accurately. With the increase of the number of important nodes of fluctuation, nodes 18, 19, 29, 32, 12, 15, 16, 6, 8 and 3 will also have cascade fluctuation, that is to say, with the increase of the number of important nodes of fluctuation, the flow rate of ethylene chlorination reaction, oxychlorination reaction and crude dichloroethane purification process is extremely easy to be abnormal, and the flow rate of materials in the reaction process needs to be strictly monitored.

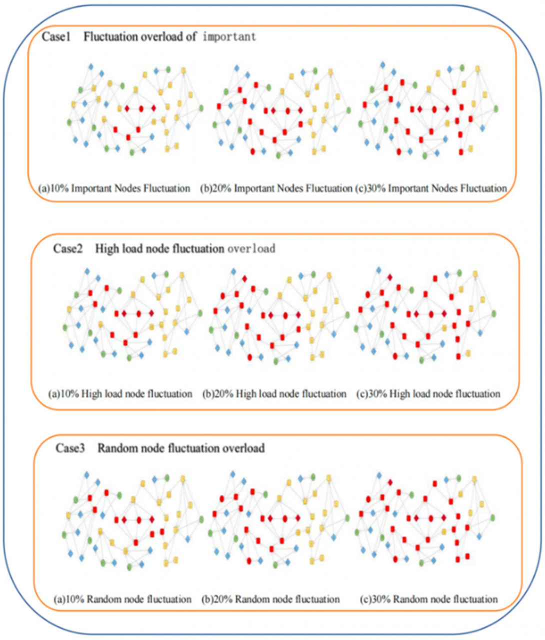


Figure 6. Cascading Volatility Risk Propagation Path

5. Conclusion

Based on the complex network theory, combined with the actual production process, the network model of vinyl chloride production process is established, and on the basis of this model, the cascade fluctuation propagation model is further constructed based on the cascade fluctuation theory, and the cascade fluctuation propagation path of vinyl chloride production process network is studied by using this model. The main conclusions are as follows:

(1) In the production process of vinyl chloride, the reaction pressure, temperature and flow rate of reactants are prone to cascade fluctuations when crude vinyl chloride is refined. The parameters on this path should be the main focus of monitoring to ensure that timely measures can be taken to prevent the spread of cascade fluctuations and ensure the safe and stable operation of the vinyl chloride production process.

(2) In the establishment of complex network model, we not only consider the direction of the network, topological properties and the risk of materials, but also comprehensively compare and analyze the fluctuation risk propagation path under different fluctuation overload modes, which can better predict the cascade risk propagation path in the process of vinyl chloride production, and provide a reliable theoretical basis for the development of monitoring plan in the process of vinyl chloride production, and accurately and timely block the propagation of failure.

Acknowledgment

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