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Risk Variable Identification of Synthetic Ammonia Process Based on Complex Network Analysis and Symbolic Digraph

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Abstract: Ammonia synthesis is one of the most important inorganic production processes in chemical industry, and the identification of risk variables in ammonia synthesis process is the key link to realize its process control and optimization. Therefore, this paper focuses on the identification of key variables in the process of synthetic ammonia. The method of combining complex network analysis and symbolic digraph for the first time is applied to the ammonia synthesis process, and the conclusion obtained by this method is compared with that obtained by using HAZOP to identify the risk of ammonia synthesis process. The results show that the combination of complex network analysis and symbolic digraph can be used as a tool to identify the risk variables in the process of ammonia synthesis, and this method integrates subjective and objective factors, and the obtained weights are more scientific and practical, thus improving the accuracy of evaluation.

1. Introduction

At present, the scale of chemical production is expanding day by day, because the equipment, instruments, technological process and production environment that constitute the chemical process system are becoming increasingly complex, and the conditions for chemical production are usually high temperature, high pressure and toxic[1]. Once an accident happens, it will inevitably endanger the safe and stable operation of the whole production process. Therefore, it is particularly important to effectively identify the variables that may be at risk in the chemical production process, so as to realize the safety assessment of the chemical process. In recent years, many researchers have done a lot of research on the identification of key variables in the chemical process. He[2] put forward an RB-PLSIELM model, which combines the improved extreme learning machine (RB) with the partial least squares (PLSIELM) and the nonlinear model to identify the key risk variables in the chemical process. The actual case analysis proves that the proposed method has high accuracy and stability. S.J. Watts et al[3] put forward a measurement method for identifying key risk variables in chemical process, which applies the degree of inseparability of subspaces of variable subsets to provide reasonable estimation of the monitoring performance of variable subsets, and verifies the effectiveness of this method in identifying correct key variables through a process case of TE. In addition, in recent years, complex networks have been rising rapidly, and the identification of key nodes in complex network models has attracted the attention of many scholars. Complex network is an effective tool to describe and analyze complex systems from the aspects of correlation and multi-scale[4-5]. In recent years, many scholars have used the model of complex network to describe related variables in security analysis, and then turned the problem of risk identification into the problem of network analysis. Therefore, in addition to the above research methods, researchers also apply complex network theory analysis to the identification of key variables in chemical processes. For example, Jiaye Yan et al[6] studied the structural identification of unknown complex dynamic networks with complex coupling; Cai et al[7] combined complex network analysis with principal component analysis, established a chemical process network model and monitored the chemical process, and then detected the fault source of the chemical process system. Similarly, the SDG method has developed rapidly in recent years because of its high value in practical industrial production. The main aspects of SDG research include risk propagation mechanism in complex systems and the development of modeling theory based on in-depth knowledge of complex systems [8]. The technical model has been widely used in many fields and achieved good results. For example, Mobed et al[9] used SDG modeling to configure sensors in chemical process system, and introduced fault evolution sequence and amplitude ratio information to enhance sensor positioning, so that abnormal variables in the system could be identified early; JLiu et al[10] proposed a fault diagnosis method based on probability extended digraph and fault index reasoning, and simulated the TE process as an example. The diagnosis method has high fault resolution in fault location. Dong Yuxi et al[11] considered the change characteristics of the correlation of system variables, calculated the network statistical index with Pearson correlation coefficient (PCC), and combined with SDG model, created the optimal PCC-SDG network and diagnosed the risk of TE process. This method accurately identified the risk types and had high accuracy.

Ammonia synthesis is one of the most important inorganic production processes in chemical industry, and the identification of risk variables in ammonia synthesis process is very important for its safety assessment. Ammonia synthesis mainly takes coal and natural gas as raw materials, and purifies the crude raw gas through shift process, desulfurization and decarbonization process and gas refining process. The purified gas is compressed by compressor, and finally enters the reactor to make the required finished ammonia[12]. As most domestic synthetic ammonia industrial processes involve high temperature and high pressure, there are also many potential safety hazards in the whole process. It is of great significance to identify the key variables that may cause failures in the synthetic ammonia process in time to ensure the long-term stable operation of the synthetic ammonia production plant, and then to ensure the safety of employees' lives and property.

In order to ensure the long-term stable operation of the ammonia plant. In China, Zhang Feng et al[13] took the two-stage ammonia separation process of medium-pressure synthesis as the research object, and made hazard analysis on five aspects of the process: medium, process, equipment, control and system. Qi Haitao et al[14] used HAZOP method to analyze the meaningful deviation in ammonia converter, the causes of deviation and possible consequences, and put forward corresponding countermeasures; Qin Yan et al[15] put forward SDG method based on complex network target control theory for the identification of risk variables in chemical process, and verified this method by taking synthetic ammonia process as one of the cases. Abroad, LvC, WuZ, etc[16] have built 17-S risk evaluation indexes and established a multi-level risk evaluation standard system from three aspects: safety production conditions, safety technology and safety management. ZLA, WTA et al[17] put forward an intelligent quantitative risk assessment method (DYN-LSTM-QRA) for ammonia synthesis process based on dynamic mechanism model, and applied this method to the leakage accident in ammonia synthesis process to assess the potential accident risk caused by dynamic chemical conditions.

Although considerable research has been carried out on the identification of risk variables in synthetic ammonia process at home and abroad, it is still a blank to combine complex network analysis with SDG modeling to identify risk variables in synthetic ammonia process. This paper focuses on the identification of risk variables in synthetic ammonia process. In order to improve the accuracy and reliability of risk variable identification, this paper first applies complex network analysis and SDG modeling to the field of risk variable identification in synthetic ammonia process.

Traditional HAZOP and SDG modeling are widely used as risk identification methods. HAZOP risk identification is characterized by its strong subjectivity, which relies on the experience of experts by using the deviation of leading words. SDG modeling method for risk identification is an important field of security technology. SDG method can use nodes and branches to describe complex systems as qualitative network models. Combining complex network analysis with SDG modeling makes up for the objectivity deficiency of traditional HAZOP identification methods and improves the comprehensiveness and accuracy of risk identification[18-23]. At present, some researchers have applied the method of complex network analysis and SDG modeling to the risk identification of synthetic ammonia process, but it is only one of the cases to verify the risk identification method of chemical process, yet no research has been found which focuses on the risk variable identification of synthetic ammonia process[24-28].

In this paper, complex network analysis and SDG modeling are used to identify the risk variables of synthetic ammonia process. The research process builds a complex network model based on the SDG model of synthetic ammonia chemical process, and identifies the key risk variables of synthetic ammonia process by TOPSIS analysis method. Finally, the results obtained by combining complex network analysis with SDG modeling are compared with those obtained by traditional HAZOP method.

Compared with previous studies, the innovations of this paper mainly include the following two points:

(1) Focus on the identification of risk variables in synthetic ammonia process for the first time.

(2) In order to realize the comprehensive and accurate identification of risk variables in synthetic ammonia process, the method of combining complex network analysis with SDG modeling is applied to the identification of risk variables in synthetic ammonia process for the first time.

2. SDG Model and Complex Network Model Construction of Ammonia Synthesis Process

2.1 SDG Model of Synthetic Ammonia

In the ammonia synthesis process, coal and natural gas are used as raw materials. Firstly, raw materials such as coal and natural gas are processed and converted into crude raw materials containing nitrogen and hydrogen. Then, the crude raw materials are desulfurized and decarbonized to obtain pure nitrogen-hydrogen mixture, which is compressed by a compressor and finally fed into a reactor to produce the required finished ammonia. It consists of four types of units: ammonia converter, heat exchanger, gas-liquid separator and compressor. Because of the complexity of the three-stage reaction in the synthetic tower, the whole reaction effect in the tower is difficult to be simulated by a single reactor model. Therefore, three reactors and two heat exchangers are integrated to represent the synthetic tower. The specific ammonia synthesis process is shown in Figure 1. According to the ammonia synthesis process, the related variables in the system are defined. See Table 1 for details.

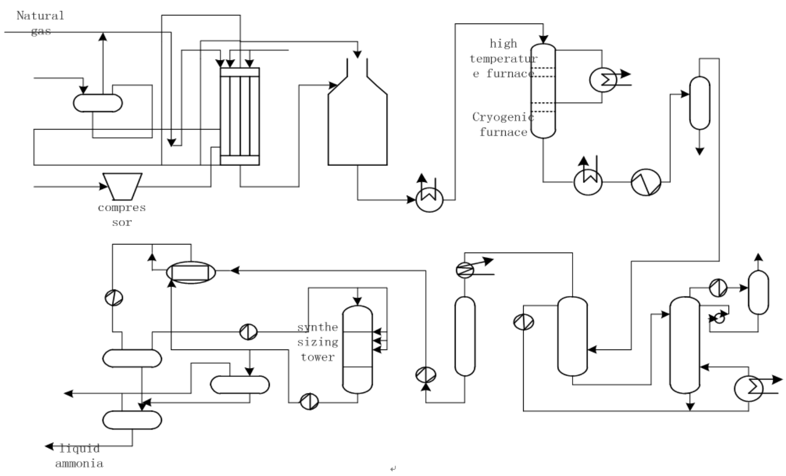

Figure 1: Flow chart of synthetic ammonia process

Table 1: Definition of variables in synthetic ammonia process

node	name	node	name	node	name
1	Natural gas inlet flow	11	Compressor flow	21	Liquid level of synthetic tower
2	Soft water inlet flow	12	Inlet pressure of primary reformer	22	Synthetic tower temperature
3	Steam valve	13	Compressor outlet pressure	23	Synthetic tower pressure
4	the steam flow meter	14	Outlet pressure of secondary reformer	24	Reaction logistics
5	Temperature of primary reformer	15	Temperature of converter cooler	25	Liquid ammonia storage tank
6	Flow rate of primary reformer	16	Gas outlet temperature of shift tower	26	Boiler water preheater
7	Secondary reformer flow rate	17	Absorption tower liquid level	27	Low furnace inlet temperature
8	Pressure of primary reformer	18	gas-liquid separator	28	Low shift gas outlet composition
9	Temperature of secondary reformer	19	Methanation furnace	29	Natural gas valve
10	Secondary reformer pressure	20	ammonia compressor	30	Air valve

SDG model is a way to describe large complex systems, which consists of nodes and directed edges, where nodes represent system variables. If one variable deviates, it will affect another variable. Then, these two variables are connected by directed edges, and the direction is from the cause to the result, and the positive and negative effects of the influences are represented by "+"and "-"respectively.

Through the relationship between the variables in the synthetic ammonia process and the components of the valve, the variable relationship in the synthetic ammonia process is expressed (see Appendix Table 2 for details) and the SDG model of the synthetic ammonia process is obtained, as shown in Figure 2.

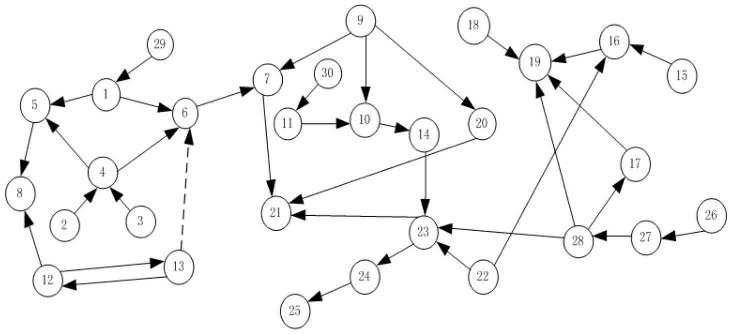

Figure 2: SDG model of ammonia synthesis process

2.2 Building Complex Network Based on SDG Model of Synthetic Ammonia

The variables expressed in the SDG model of ammonia synthesis process shown in fig. 3 and the relationships among variables are regarded as nodes and edges in the network, respectively, and the adjacency matrix A of the network is established. The elements in the matrix A represent the correlation between nodes I and J in the network, and when there is correlation between nodes I and J, the elements in the matrix are equal to 1; On the contrary, = 0; And when i=j, =0. The adjacency matrix of the synthetic ammonia network is as follows:

$$A_1 = \begin{bmatrix}
0&0&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&1&1&0&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
1&0&0&1&0&1&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
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0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{bmatrix}$$

According to the adjacency matrix, the network structure diagram of synthetic ammonia is obtained by using Gephi software, as shown in Figure 3.

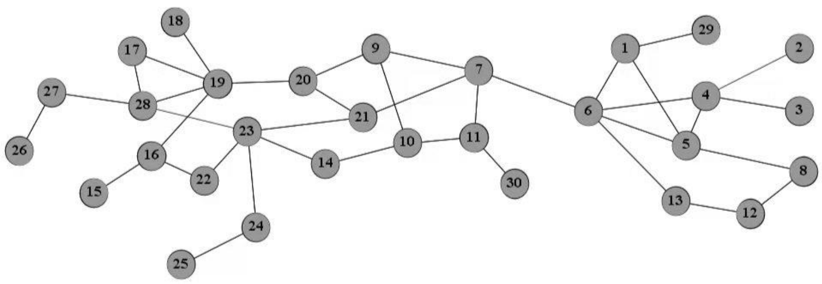

Figure 3: Network structure diagram of ammonia synthesis process

3. Identification of Key Process Variables of Ammonia Synthesis Based on Complex Network

3.1 Select the Importance Evaluation Index of Synthetic Ammonia Network Nodes.

The importance of a single node in a synthetic ammonia network is usually closely related to its overall structure. Therefore, the integrity of the network should not be damaged when identifying the key nodes in the synthetic ammonia network. In addition, the single index has some limitations and one-sidedness in the calculation of network topology analysis, which makes it difficult to quantify the importance of a single node in the whole network. Considering the above factors and following the principles of rationality, feasibility, purpose and comprehensiveness, point centrality, near centrality, intermediate centrality, feature vector centrality and structural hole are selected as the indexes for comprehensive evaluation of the nodes in the ammonia synthesis network (see Appendix (1)~(6) for the calculation formulas of the indexes). The calculation results of each index of the nodes in the ammonia synthesis process network are shown in Table 3.

Table 3: Results of each index of synthetic ammonia network node

node	DC	CC	FBC	EC	C
1	3	114	28	0.62	0.6
2	1	140	0	0.214	1
3	1	140	0	0.214	1
4	4	112	55	0.693	0.47
5	4	110	32	0.813	0.53
6	5	90	192	1	0.38
7	4	80	210	0.734	0.25
8	2	135	4	0.318	0.5
9	3	89	49	0.477	0.333
10	3	100	24	0.343	0.333
11	3	102	37	0.368	0.333
12	2	140	1	0.214	0.5
13	2	115	24	0.375	0.5
14	2	104	18	0.264	0.5
15	1	147	0	0.078	1
16	3	119	31	0.251	0.333
17	2	120	0	0.294	1.125
18	1	127	0	0.154	1
19	5	99	78	0.499	0.3
20	3	91	69	0.465	0.333
21	3	80	137	0.529	0.333
22	2	106	19	0.236	0.5
23	5	84	150	0.511	0.21
24	2	110	28	0.175	0.5
25	1	138	0	0.054	1
26	1	152	0	0.048	1
27	2	124	28	0.154	0.5
28	4	98	72	0.451	0.47
29	1	142	0	0.192	1
30	1	130	0	0.114	1

3.2 Determination of Index Weight of Ammonia Synthesis Network Nodes

The objective weighting method of principal component analysis is used to determine the index weight of synthetic ammonia network nodes. This method determines the index weight value through the correlation between each index and the variation degree of each index result value, which not only avoids the deviation caused by human factors, but also eliminates the mutual influence among evaluation indexes (see Appendix (7)~(10) for specific algorithm steps).

After the index matrix of synthetic ammonia network is standardized by principal component analysis, the correlation coefficient matrix R can be obtained.

$$R = \begin{bmatrix} 1 & -0.7956 & 0.7737 & 0.8494 & -0.7909 \\ -0.7956 & 1 & -0.7867 & -0.7050 & 0.8053 \\ 0.7737 & -0.7867 & 1 & 0.7521 & -0.6402 \\ 0.8494 & -0.7050 & 0.7521 & 1 & -0.6017 \\ -0.7909 & 0.8053 & -0.6402 & -0.6017 & 1 \end{bmatrix}$$

The eigenvalue of the matrix r can be obtained by matlab software:

$$\overline{W_i} = [W_{DC}\ W_{CC}\ W_{FBC}\ W_{EC}\ W_C]$$

$$=[0.0192\ 0.0311\ 0.0585\ 0.0902\ 0.8010]$$

3.3 Identification of Key Variables in Synthetic Ammonia Network Model Based on TOPSIS Method

Table 4: Weighted Normalization Matrix Y of Synthetic Ammonia Network

	1	2	3	4	5
1	0.0115	0.0233	0.0078	0.0559	1.5019
2	0.0038	0.0286	0	0.0193	0.9011
3	0.0038	0.0286	0	0.0193	0.9011
4	0.0154	0.023	0.0152	0.0625	1.9176
5	0.0154	0.0224	0.0088	0.0733	1.7005
6	0.0192	0.0183	0.0532	0.0902	2.371
7	0.0154	0.0165	0.0585	0.0662	3.6045
8	0.0077	0.0277	0.0011	0.0287	1.8023
9	0.0115	0.0183	0.0135	0.043	2.7074
10	0.0115	0.0205	0.0067	0.0309	2.7074
11	0.0115	0.0208	0.0103	0.0332	2.7074
12	0.0077	0.0286	0.0003	0.0193	1.8023
13	0.0077	0.0236	0.0067	0.0338	1.8023
14	0.0077	0.0211	0.005	0.0238	1.8023
15	0.0038	0.0302	0	0.007	0.9011
16	0.0115	0.0243	0.0087	0.0226	2.7074
17	0.0077	0.0246	0	0.0265	0.801
18	0.0038	0.0261	0	0.0139	0.9011
19	0.0192	0.0202	0.0216	0.045	3.0038
20	0.0115	0.0187	0.0193	0.0419	2.7074

It is convenient and effective to apply TOPSIS (Approximate Ideal Sorting Method) multi-attribute decision method to comprehensively evaluate several indexes of the importance of ammonia network nodes. Its basic idea is to treat each node in ammonia network as an object to be evaluated, and the importance evaluation indexes of several nodes as attributes of each object, and further transform the node importance evaluation into a multi-attribute decision problem. Finally, by calculating the closeness between each index of the object to be evaluated and the ideal solution, the ranking results are used as the basis for judging the importance degree of nodes (see Appendix (11)~(18) for the detailed calculation process of TOPSIS method).

TOPSIS method is applied to calculate the node importance of ammonia synthesis process network;

(1) From the description of index types in the appendix, it can be known that the center of point degree (DC), the center of approach degree (CC), the center of intermediate degree (FBC) and the center of feature vector (EC) belong to the benefit type index, and the structural hole (C) belongs to the cost type index. Calculate the index matrix of synthetic ammonia network according to formulas (11) and (12) to obtain the normalized matrix P, and then combine the normalized matrix P with the weight coefficient obtained by principal component analysis to obtain the weighted normalized matrix Y as shown below. Due to the limited space, only 20×5 matrices are listed in Table 4 for the weighted normalization matrix of ammonia synthesis network, and the weighted normalization values of other nodes are shown in Appendix.

(2) Further, the positive ideal solution and negative ideal solution of the synthetic ammonia network are obtained by formulas (14) and (15).

$$A^{+}=[0.0192\ 0.0311\ 0.0585\ 0.0902\ 4.2934]$$

$$A^{-}=[0.0038\ 0.0165\ 0\ 0.0043\ 0.801]$$

(3) Finally, formulas (16), (17) and (18) are applied to calculate the distance and closeness of each index of synthetic ammonia network to positive and negative ideal solutions, respectively. The evaluation results are shown in Table 5 below.

Table 5: TOPSIS method to evaluate the results of each node of ammonia synthesis network

node	D_i^+	D_i^-	C_i	node	D_i^+	D_i^-	C_i
1	2.7922	0.7029	0.2011	16	1.5882	1.9065	0.5455
2	3.3935	0.102	0.0292	17	3.4935	0.0239	0.0068
3	3.3935	0.102	0.0292	18	3.3936	0.101	0.0289
4	2.3763	1.1183	0.32	19	1.291	2.2033	0.6305
5	2.5934	0.9023	0.2581	20	1.5873	1.9069	0.5457
6	1.9224	1.5733	0.4501	21	1.5868	1.9073	0.5459
7	0.6894	2.8048	0.8027	22	2.4927	1.0014	0.2866
8	2.4926	1.0016	0.2867	23	0.0493	3.4929	0.9861
9	1.5874	1.9068	0.5457	24	2.4928	1.0014	0.2866
10	1.588	1.9066	0.5456	25	3.3938	0.1008	0.0289
11	1.5878	1.9066	0.5456	26	3.3939	0.1012	0.029
12	2.4928	1.0014	0.2866	27	2.4928	1.0014	0.2866
13	2.4923	1.0017	0.2867	28	2.3798	1.1142	0.3189
14	2.4926	1.0015	0.2866	29	3.3936	0.1017	0.0291
15	3.3938	0.1011	0.0289	30	3.3937	0.1008	0.0289

According to the order of importance of the closeness of each node in the synthetic ammonia network obtained in Table 4, it can be concluded that node 23, node 7, node 20 and node 22 are the key nodes of the synthetic ammonia network model, which correspond to the four variables of synthetic tower pressure, secondary reformer flow rate, ammonia compressor and synthetic tower temperature in the synthetic ammonia process. This conclusion coincides with Qi Haitao's conclusion that "the temperature and pressure of the synthetic tower are the main factors for its safe operation" by applying HAZOP technology to the hazard identification of ammonia synthesis tower. In addition, the flow rate of the secondary reformer and the ammonia compressor also have a significant impact on the stable operation of the ammonia synthesis process, which is a variable prone to problems.

4. Conclusion

(1) Based on the SDG model of synthetic ammonia process and the further complex network model of synthetic ammonia, this paper analyzes the complex network model of synthetic ammonia, selects five indexes of network nodes, such as point centrality, near centrality, intermediate centrality, eigenvector centrality and structural hole, and identifies the key variables of synthetic ammonia process by combining principal component analysis and TOPSIS method. They are the pressure of the synthetic tower, the flow rate of the secondary reformer, the ammonia compressor and the temperature of the synthetic tower, which improves the comprehensiveness and accuracy of identifying the key variables of the synthetic ammonia process[29].

(2) Identifying the key variables in the ammonia synthesis process from the perspective of complex network model analysis not only provides theoretical support for predicting and controlling the risks in the ammonia synthesis process in advance, but also has certain reference significance for maintaining the safety and stability of other large-scale complex processes. Next, we can further study the cascading failure propagation caused by the failure of key variables in the ammonia synthesis process system, and provide more effective theoretical decision support for the risk prediction and prevention of the ammonia synthesis process system[30].

(3) Applying the previous research on the identification of key risk variables in chemical process to the analysis of complex network model based on synthetic ammonia process has an important role in ensuring the safe and stable operation of synthetic ammonia process, but there are still some shortcomings. The research methods mentioned above are based on the topological structure and statistical characteristics of complex networks to identify key nodes in the system, but the importance of driving nodes in the network is not considered from the perspective of complex network control theory[31]. With the continuous development of synthetic ammonia process system, its network model is becoming more and more complex. At the same time, monitoring based on key variables is helpful to reduce the monitoring load of the system and improve the sensitivity of the system. Therefore, how to accurately identify key variables in synthetic ammonia process needs to be improved.

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Appendix

Table 2: Relationship table of synthetic ammonia variables

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1					+	+														
2				+																
3				+																
4					+	+														
5								+												
6							+													
7																				
8																				
9							+			+										+
10														+						
11							+			+										
12								+					+							
13						-						+								
14																				
15																+				
16																			+	
17																			+	
18																			+	
19																				+
20																				
21																				
22																				
23																				
24																				
25																				
26																				
27																				
28																	+		+	
29	+																			
30											+									

Table 2: Relationship table of synthetic ammonia variables

	21	22	23	24	25	26	27	28	29	30
1									+	
2										
3										
4										
5										
6										
7	+									
8										
9										
10										
11										
12										
13										
14			+							
15										
16		+								
17										
18										
19										
20	+									
21										
22			+							
23	+			+						
24					+					
25										
26							+			
27								+		
28			+							
29										
30										

Evaluation index of node importance:

(1) Centricity of points

$$DC(i) = \frac{k_i}{N-1} \quad (1)$$

In the above formula, DC is the ratio of the number of connected nodes of node I to the maximum number of possible nodes of node I. The larger the value, the more important the node is. Is the number of nodes directly connected to node I, and n is the total number of nodes in the network.

(2) Approaching the centrality.

$$CC(i) = \frac{N-1}{\sum_{j \neq i} d_{ij}} \quad (2)$$

In the formula, CC is the reciprocal of the sum of distances from node I to other nodes in the network; Is the shortest path length between node I and node J.. The greater the CC value, the greater the degree that the node is in the center of the network, and the higher its position.

(3) Intermediate centrality

$$FBC(i) = \sum_{s<t} \frac{\widetilde{g_{st}{}^{i}}}{\widetilde{g_{st}}} \tag{3}$$

In the above formula, FBC refers to the proportion of paths passing through a node among all non-repeated paths. The larger the value, the more important the node is. Is the number of paths passing through I between nodes S and T; Are all paths between nodes S and T.

(4) Centricity of eigenvector

$$EC(i) = \lambda^{-1} \sum_{j=1}^{N} a_{ij} x_j \tag{4}$$

In the above formula, EC is the eigenvector corresponding to the maximum eigenvalue of the network adjacency matrix, and the larger its value is, the more important the node is; λ is the largest eigenvalue of adjacency matrix A; Is the eigenvector corresponding to the maximum eigenvalue λ.

(5) Structural hole

$$C(i) = \left(\sum_{j} p_{ij} + \sum_{q \neq i \neq j} p_{iq} p_{qj} \right)^2 \tag{5}$$

If there is no direct connection and indirect redundancy between two nodes in the network, the obstacle between them is the structural hole. Where q is an indirect node connecting nodes I and J; The proportion of time spent on J for node I in its total time. The smaller the value of c, the greater the degree of structural hole, and the more important the node position. (Note: This formula is the restriction degree of each index of structural hole, and the restriction degree of some nodes may be null when analyzing the related process network. At this time, the grade degree of structural hole index is selected as the result value of this index. The formula is: (6)$HI_i = \frac{\sum_j (C_{ij} / \frac{C_i}{N}) \ln(C_{ij} / \frac{C_i}{N})}{N \ln(N)}$, Degree can describe some characteristics of structural hole nodes; The higher the degree index, the more restrictive it is in a certain node's neighborhood. Type$C_{ij} = \left(p_{ij} + \sum_{q \neq i \neq j} p_{iq} p_{qj} \right)^2$, N is the number of network nodes).

Determine the weight of each index of the network:

(1) establish an evaluation index matrix

A network with n nodes, if there are m evaluation indexes of node importance, the evaluation index matrix x is:

$$X = \begin{bmatrix} x_{11} & \cdots & x_{1m} \\ \vdots & \ddots & \vdots \\ x_{N1} & \cdots & x_{Nm} \end{bmatrix} \tag{6}$$

(2) Matrix standardization

Z-score method is used to standardize data transformation.

$$Z_{ij} = \frac{x_{ij} - \overline{x_j}}{S_j} \tag{7}$$

Among them, $\overline{x_j} = \frac{\sum_{i=1}^{N} x_{ij}}{N}$, $S_j^{\ 2} = \frac{\sum_{i=1}^{N} (x_{ij} - \overline{x_j})^2}{N-1} (i = 1, \cdots, N; j = 1, \cdots, m)$ 。

(3) Find the correlation coefficient matrix R.

$$R = \frac{Z^T Z}{N-1} = (r_{ij})_{p \times p} \tag{8}$$

(4) Find the eigenvalue of matrix R.

The eigenvalue of correlation coefficient matrix R is obtained by MATLAB software. $\lambda_1, \lambda_2, \cdots, \lambda_p$, Calculate the contribution rate of each index, that is, the weight coefficient. $\overline{w_j}$.

$$\overline{w_j} = \frac{\lambda_i}{\sum_{i=1}^{p} \lambda_i} \tag{9}$$

Step of judging network node importance based on TOPSIS algorithm:

(1) Standardization of index matrix

Because there are many indexes, different dimensions and complicated relationships among them, it is necessary to standardize the indexes in order to facilitate comparison. Types of indicators can be divided into benefit-oriented indicators (the higher the index value, the stronger the ability) and cost-oriented indicators (the higher the index value, the worse the ability). According to the different types, they can be treated as formula (10) and formula (11).

$$\text{Benefit type} \quad p_{ij} = \frac{x_{ij}}{x_j^{\max}} \tag{10}$$

$$\text{Cost type} \quad p_{ij} = \frac{x_j^{\min}}{x_{ij}} \tag{11}$$

Among them, $x_j^{\max} = \max\left\{x_{ij} \mid 1 \le i \le N\right\}$, $x_j^{\min} = \min\left\{x_{ij} \mid 1 \le i \le N\right\}$. Finally, the normalized matrix is P= $(p_{ij})_{N \times m}$.

(2) Construct a weighted normalization matrix.

The weight coefficient of each index obtained by principal component analysis and matrix P constitute a weighted normalized matrix, as shown in formula (12).

$$Y = (y_{ij}) = (w_j p_{ij}) = \begin{bmatrix} w_1 p_{11} & \cdots & w_m p_{1m} \\ \vdots & \ddots & \vdots \\ w_1 p_{N1} & \cdots & w_m p_{Nm} \end{bmatrix} \tag{12}$$

Table 4: Weighted Normalization Matrix Y of Synthetic Ammonia Network

	1	2	3	4	5
21	0.0115	0.0165	0.038	0.0477	2.7074
22	0.0077	0.0218	0.0053	0.0213	1.8023
23	0.0192	0.0171	0.0415	0.0461	4.2934
24	0.0077	0.0224	0.0078	0.0158	1.8023
25	0.0038	0.0283	0	0.0049	0.9011
26	0.0038	0..0311	0	0.0043	0.9011
27	0.0077	0.0255	0.0078	0.0139	1.8023
28	0.0154	0.0199	0.0201	0.0407	1.9144
29	0.0038	0.0289	0	0.0173	0.9011
30	0.0038	0.0267	0	0.0103	0.9011

(3) Determine the positive ideal solution and the negative ideal solution and calculate the distance scale

Determine the positive ideal solution according to the matrix y A^+ And negative ideal solution A^-, See formula (13) and formula (14).

$$A^+ = \left\{ \max_{i \in K}(y_{i1}, \cdots, y_{im}) \right\} = \left\{ y_1^{\max}, \cdots, y_m^{\max} \right\} \tag{13}$$

$$A^- = \left\{ \min_{i \in K}\left(y_{i1}, \cdots, y_{im}\right) \right\} = \left\{ y_1^{\min}, \cdots, y_m^{\min} \right\} \tag{14}$$

Type, $K = \{1, \cdots, N\}$.

Use European distance formula to calculate each index. A_i To positive ideal solution A^+ And negative ideal solution A^- See formula (15) and formula (16) for the distance d of.

$$D_i^+ = \left[\sum_{j=1}^{m} \left(y_{ij} - y_j^{\max} \right)^2 \right]^{1/2} \tag{15}$$

$$D_i^- = \left[\sum_{j=1}^{m} \left(y_{ij} - y_j^{\min} \right)^2 \right]^{1/2} \tag{16}$$

(4) Calculate the closeness of each index to the ideal solution.
The calculation formula of closeness degree C is as shown in Formula (17).

$$C_i = \frac{D_i^-}{D_i^+ + D_i^-} \tag{17}$$

According to C_i The value of ranks the importance of nodes.