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Application of Artificial Intelligence in Separation Technology of Chemical Process

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Separation technology is the key in the chemical production process, and it is related to the quality and economic benefits of chemical products. Based on the artificial intelligence technology (AIT), in this paper, the synthesis problems in the separation process of the chemical production process was deeply discussed to realizes the computerization of the separation process. Besides, the case analysis was conducted. The research results show that the chemical separation process has validity, integrity and intuitive rationality. The use of AIT to develop intelligent program system can realize the smart selection of separation method, mass separating agent and separation device, etc. for the given separation problem. It can also make soring of separation points for the separation problem, provide the initial separation process, and independently implement the separation process tuning and separation integration.

1. Introduction

Chemical industry is the key industry in the national economy. As the global economic competition intensifies, the technical and economic indicators increase, and the number of non-renewable resources decreases constantly, the chemical system structure has undergone tremendous changes (Gupta et al., 2015; Eutimio et al., 2016). In the fifties, chemical engineers began to use mathematical simulation method to solve the design and development problem of the unit process, fundamentally changing the traditional design and development method, that is, progressive amplification (Wang et al., 2016). In the 1960s, people were no longer content with solving the computational problems of individual units on a computer and began experimenting with computer-based simulations of the entire chemical process system, thereby developing the chemical process simulation system (Azhin et al., 2008; Ganesapillai et al., 2016). Since the 1980s, artificial intelligence technology has entered the field of chemical engineering research. However, due to limitations in the AIT level at that time, artificial intelligence technology was not applied in depth (Jørgensen and Jensen, 2009).
The commonly used knowledge expression methods in artificial intelligence include production rule, framework structure, and semantic network etc. (Qiu et al., 2013). According to the characteristics of knowledge in different fields, proper knowledge expression method can be used to describe, and make computer code and establish the relevant knowledge base. Separation technology is very important in the chemical production process, and almost all chemical processing processes cannot go without the separation technology. The advantages and disadvantages of the separation process design directly affect the product quality, dosage and benefits of the entire chemical production process (Dubreuil et al., 2017). In the chemical separation technology, it is difficult for the traditional simulation technology to make breakthrough progress, and thus the artificial intelligence technology has a wide application prospect. Based on artificial intelligence technology, this paper carries out the thorough discussion about the synthesis problem in the chemical production separation process, and realizes the computerization of separation process, so as to provides the effective tool and method for the process design.

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2. Systematic solution to selective problem

2.1 Decomposition and knowledge structure model of selective problems

Chemical separation technology includes separation method selection, separating agent selection, and separation device selection. Most of the problems related to selectivity are not quantitative, but qualitative, which cannot be described by numerical values and algorithms. The solving process of the selective problem is to search the selected object space and test the constraint set. Due to the characteristics of the chemical industry itself, the objective facts, empirical rules and quantitative model involved are very complicated. Objective facts include physical data, separating agent, separation methods, and separation device; empirical rules include empirical summary and inferences; quantitative model includes mathematical model etc. There is a large amount of knowledge involved in the selective problem, and the knowledge rules are disorderly. Fig.1 shows the classification tree diagram of separation process. The separation process includes mechanical separation and diffusion separation, where the mechanical separation includes suspension separation, emulsion separation, foam liquid separation, dust-laden gas separation, and fog gas separation; diffusion separation includes liquid phase component separation and gas phase component separation. The separation method of liquid phase components includes flash distillation, ordinary distillation, liquid-liquid extraction, extractive distillation, azeotropic distillation and crystallization etc.

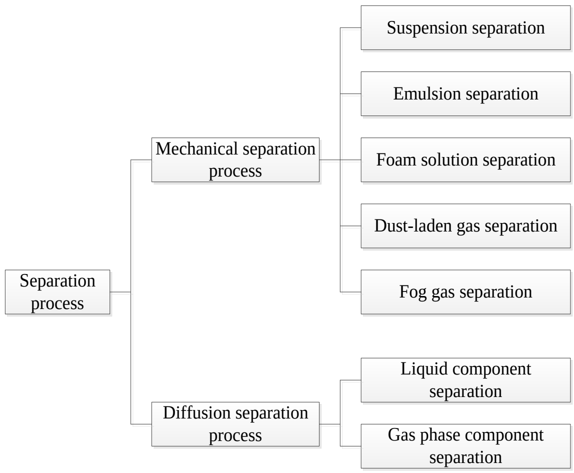


Figure 1: Separation process classification tree

2.2 Selective expert system design method

Table1: Azeotropic binary mixture with the highest boiling point

A	B	Mol% A	Temperature /℃	Pressure/mm
H_2O	Hydrofluoric acid (HF)	64.3	119	
H_2O	Hydrochloric acid(HCl)	87.8	109	
H_2O	Perchloric acid ($HClO_4$)	31.9	202	
Trichloromethane	Acetone	64.4	63.5	
Formic acid	3-pentone	47.9	104.4	760
Formic acid	2-pentone	46.9	104.3	
Phenol	Cyclohexanol	89	181.45	
Phenol	Benzaldehyde	53	184.5	
O-cresol	Acetophenone	23	202.6	
M-cresol	Acetophenone	53	208	

The empirical rules related to the selective problem includes two types of models: hierarchical and relational. The hierarchical design method can decompose the problem into several parts and then resolve each part separately. According to the idea of hierarchical design, the design object system can be decomposed into user consultation subsystem and expert knowledge acquisition subsystem: the user consultation subsystem includes identifying separation points, consulting knowledge bases, knowledge list, and deleting knowledge etc.; the expert knowledge acquisition subsystem includes rule base maintenance and fact base maintenance, which are further divided into establishment of knowledge base, storage of knowledge base, adding knowledge, modification of knowledge, and help information. The selection rule has an important influence on the chemical separation process. The storage of the rules should follow the order of the facts in the preceding rule and the order of the rules themselves, e.g., Table 1 lists the azeotropic binary mixture with the highest boiling point, and azeotropes do not form with a boiling point difference >30°C according to empirical standards, so the system can determine whether the object is a member of the table according to Table 1, and if so, it is determined as azeotrope.

3. Establishment of rule model for artificial intelligence separation technology

3.1 Intelligent solving method for system synthesis problems

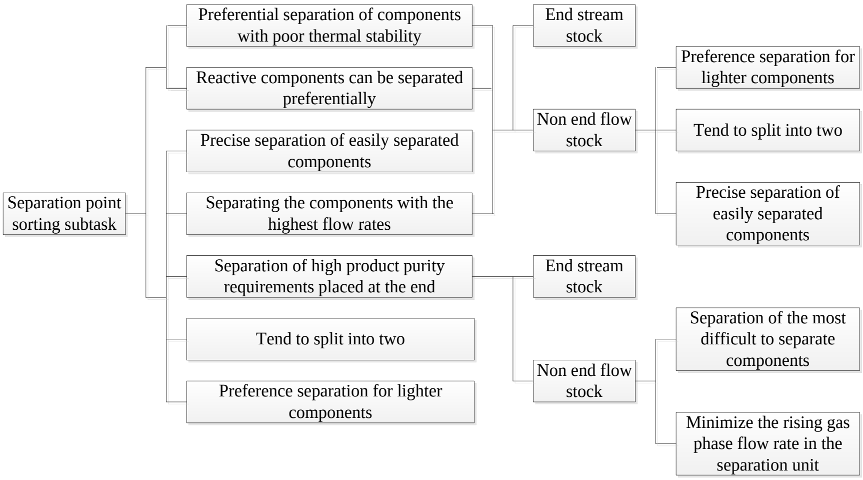


Figure 2: Exponential structure for sorting of separation points

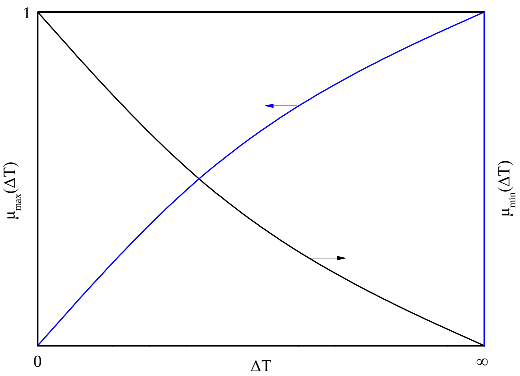
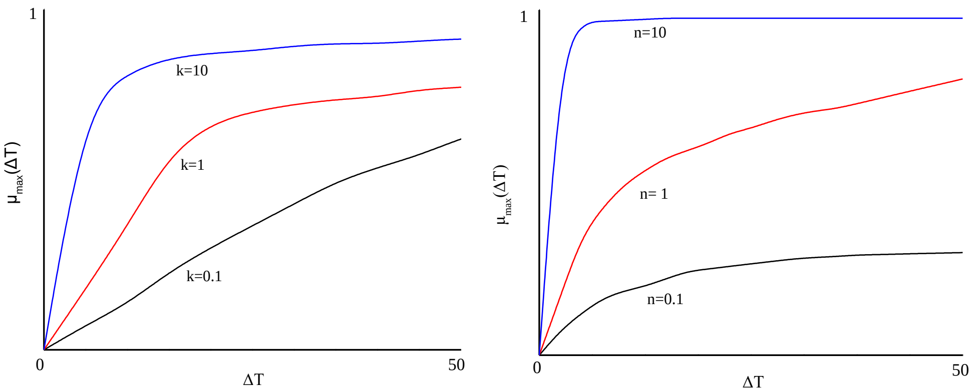


Figure 3: Relationship between μ(ΔT) and ΔT

The synthesis problems of system in the chemical separation process include three parts: separation point sorting, separation process tuning, and separation process energy integration. According to given system input and output conditions and characteristics of system requirements, it is determined that the system can reach the optimal structure, and the state tree model can be used for solving process. The paralleling conflicts between the rules related to the sorting of separation points can be resolved to a certain extent by the method of ordinal heuristics. Fig.2 shows the exponential structure for the sorting of separation points. It can be seen that preferential separation of poor thermal stability components and possibly reacting components are preferentially removed as a group; according to the separation rules: easily separated components are separated preferentially, the components with the highest flow rate are separated preferentially, and the components with high purity requirements are finally separated; besides, the separation with a tendency to be split into two isn't contradictory from the rules of priority separation of lighter components, and the separation process must be based on actual control rules. These rules have a certain degree of fuzzy quantification, the meaning of the rules itself is clear, and the application of the edge has ambiguity, which can be deduced on the basis of the membership function of the fuzzy model. The domain of the membership degree derivation model in this paper is the boiling point difference ΔT. The larger ΔT is, the higher the credibility of the key components is, the higher the credibility is. The membership function is shown in formula 1 and 2. Fig.3 shows the relationship between μ(ΔT) and ΔT. Fig.4 shows the influence of the k and n values on the membership function. The values of k and n are related to the dimension of ΔT.

$$M_{max}(\Delta T)=\frac{k\Delta T^n}{1+k\Delta T^n} \tag{1}$$

$$M_{min}(\Delta T)=1-\mu_{max}(\Delta T) \tag{2}$$



(a)n=1 (b)k=1

Figure 4: The Influence of k and n on the Membership Function

3.2 Fuzzy model with uncertainty of production rule

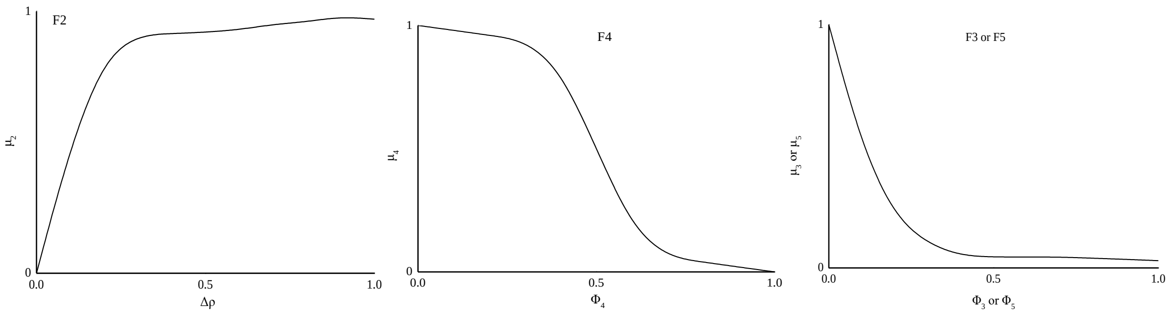


Figure 5: F2-F5 membership function

In the separation process, the products with high requirements for separation purity is difficult to separate, with a great influence on the separation points sorting. Uncertainty of separation rules includes uncertainty of facts, uncertainty of conclusions, and uncertainty of multiple rules supporting the same fact. It can be supposed that the degree of membership of each rule is one, and the credibility for the conclusions of each rule is equal to the membership degree of its premise. Then, F2 indicates the relatively high purity; F3 the relatively large flow rate; F4 relatively easy to separate, and F5 indicates that the sums of the mole fractions of light and heavy components above and below the separation point are very close. The membership function of the fact F2-F5 is shown in Formula 3-6, and the corresponding functional relationship is shown in Fig. 5.

$$\mu_2=\frac{100\Delta\rho^{1.903}}{1+100\Delta\rho^{1.903}} \tag{3}$$

$$\mu_3=\frac{1}{1+100\Phi_3^2} \tag{4}$$

$$\mu_4=\frac{1}{1+100\Phi_4^{6.644}} \tag{5}$$

$$\mu_5=\frac{1}{1+100\Phi_5^2} \tag{6}$$

4. Integrated system of chemical separation process and examples

4.1 Separation process tuning and thermal integration

The tuning method of the chemical separation process includes the three elements: the initial separation process, the tuning rules and the tuning strategy, satisfying the three rules of validity, completeness and intuitive rationality. The priority separation of the easily separated components is related to the sorting of the separation points. According to the three rules, the order and type of the separation points in the separation process are adjusted, and the separation process tuning is maximized. Adjusting the separation method and the order of the separation points is the premise to achieve a good tuning strategy. If the tuning problem and the separation problem are determined, the separation point sorting and separation method selection will be alternated to improve the tuning efficiency. In the chemical production process, the heat integration methods of separation include heat integration of the separation unit itself, heat integration between the separation units, and thermal integration of the separation process and reaction process.

4.2 Separation process integrated system SEPSES and application example

Table 2: Inlet stream composition, composition, temperature, and pressure

	Components	Composition	Literature value	Calculated value	Temperature/K	Pressure/MPa
A	Ethane	0.18				
B	Propylene	0.16	3.4	3.46		
C	Propane	0.18	1.21	1.20	311	0.1
D	1-butene	0.16	2.6	3.00		
E	N-butane	0.16	1.13	1.20		
F	N-pentane	0.16	3.18	3.31		

Table 3: Determine the degree of membership of each rule at each separation point

Rule	1	2	3
2	0.21	0.21	0.21
3	0.21	0.21	0.21
4	0.91	0.88	0.80
5	0.51	0.40	0.64
6	0.21	0.21	0.21

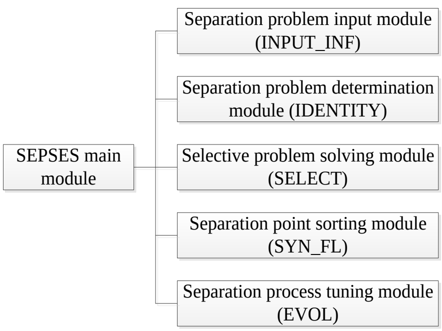


Figure 6: SEPSES main module composition

Artificial intelligence technology has been applied in chemical separation process, separation tuning, and separation integration. An artificial intelligence language has been used to develop the intelligent program system, namely SEPSES system. This system can realize intelligent selection of separation methods, mass separation agents and separation devices for any given separation problem. It can also sort separation problems by separation points, give an initial separation process and autonomously realize the separation process tuning. Fig.6 shows the composition of the main module in SEPSES. It consists of five parts: the separation problem input module, the separation problem determination module, the selection problem solving module, the separation point sorting module, and the separation process tuning module. Table 2 shows the components, composition, temperature, and pressure of the inflow, which were solved using an artificial intelligence program system. The degree of membership of each rule when determining the separation point is shown in Table 3. The SEPSES system was used to reason and select the separation method, and the chemical products in Table 2 can be separated by common distillation.

5. Conclusion

Based on the artificial intelligence technology, this paper deeply discusses the synthesis problems in the separation process of the chemical production process, realizes the computerization of the separation process, and provides effective tools and means for process design. The specific conclusions are as follows:

(1) System synthesis problems in the process of chemical separation include three parts: separation point sorting, separation process tuning, and separation process energy integration.

(2) In the separation process, it is difficult to separate the products with high separation purity requirements, which has a great influence on the sorting of separation points. The uncertainty of the separation rules includes the uncertainty of the facts, the uncertainty of the conclusions, and uncertainty of multiple rules supporting the same fact.

The artificial intelligence language was used to develop an intelligent program system that can intelligently select the separation method, mass separation agent, and separation device for any given separation problem. It can also make separate points sorting for the separation problem, give the initial separation process, and autonomously implement the tuning and optimization of separation process.

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References

Azhin M., Kaghazchi T., Rahmani M., 2008, A review on olefin/paraffin separation using reversible chemical complexation technology, Journal of Industrial & Engineering Chemistry, 14(5), 622-638, DOI: 10.1016/j.jiec.2008.04.014.

Dubreuil M.F.S., Servaes K., Ormerod D., Houtven D.V., Porto-Carrero W., Vandezande P., 2017, Selective membrane separation technology for biomass valorization towards bio-aromatics, Separation & Purification Technology, 178, 56-65, DOI: 10.1016/j.seppur.2016.12.033.

Núñez † E.G.F., Barchi † A.C., Ito S., Escaramboni B., Herculano R.D., Mayer C.R.M., 2016, Artificial intelligence approach for high level production of amylase using rhizopus microsporus, var. oligosporus, and different agro-industrial wastes, Journal of Chemical Technology & Biotechnology, 92(3), 684-692, DOI: 10.1002/jctb.5054.

Ganesapillai M., Singh A., Simha P., 2016, Separation processes and technologies as the mainstay in chemical, biochemical, petroleum and environmental engineering: a special issue, Resource-Efficient Technologies, 2(Suppl 1), S1-S2, DOI: 10.1016/j.reffit.2016.09.002.

Gupta S., Basant N., Rai P., Singh K.P. 2015, Modeling the binding affinity of structurally diverse industrial chemicals to carbon using the artificial intelligence approaches, Environmental Science & Pollution Research, 22(22), 17810-17827, DOI: 10.1007/s11356-015-4965-x.

Jørgensen K, Jensen L.S., 2009, Chemical and biochemical variation in animal manure solids separated using different commercial separation technologies, Bioresource Technology, 100(12), 3088-3096, DOI: 10.1016/j.biortech.2009.01.065.

Qiu W., Xu L., Chen C.C., Paul D.R., Koros W.J., 2013. Gas separation performance of 6fda-based polyimides with different chemical structures. Polymer, 54(22), 6226-6235, DOI: 10.1016/j.polymer.2013.09.007.

Wang K., Yu Q., Zuo Z., Hou L., Qin Q., 2016, Redox performance of cu-based oxygen carrier used in chemical looping air separation combined oxy-fuel combustion technology, Applied Thermal Engineering, 98, 440-448, DOI: 10.1016/j.applthermaleng.2015.11.097.