

Process Simulation and Analysis of Aromatics Extraction by Sulfolane*

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ABSTRACT A special process flowsheeting system for aromatics extraction by sulfolane is developed based on the systematic study on this process. The software has been successfully applied in the process analysis and design for commercial aromatics plants in China.

1. Background

The process of aromatics extraction by sulfolane is developed to recover high purity aromatics from aromatic-rich reformat or hydrotreated pyrolysis gasoline^[1]. It has many advantages and has been used all over the world. However, there are still some flaws in the original design of sulfolane unit^[2]. Extensive analyses show that it is difficult to simulate the process accurately because of the complexity and non-ideality of the system, lack of thermodynamic and dynamic data, and the sophisticated flowsheet structure. Therefore, some commercial process flowsheeting software can not simulate this process very well.

2. Simulation Software

In order to perform operation analysis and optimal design of this process, a special process flowsheeting system for Aromatics Extraction by Sulfolane is developed. This software has several advantages:

- (1) Fundamental data and design methods are reliable. This software is developed based on systematic study completed by Solvent Extraction Lab, State Key Lab of Chemical Engineering in China. The study mainly includes determination of physical properties, thermodynamics, and investigation on the performance and design of extraction column^[3-5].
- (2) It can be used to perform not only the process simulation but also the equipment design. Appropriate models of various process units are established. Efficient algorithms are used to make the calculation faster and numerically more stable^[6].

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After getting the results of process simulation, the intelligent equipment design^[7] can be performed.

- (3) A non-equilibrium stage model of the extraction column is introduced to make the simulation more strict and accurate. Although the equilibrium stage model is widely used for chemical engineers, it suffers from the drawback that the equilibrium is never achieved in a practical tray of separation columns and the empirical tray efficiencies must be used to correct the departures from equilibrium. Because the tray efficiencies vary from stage to stage within a column, as well as from component to component on a single stage, the assumption of constant efficiency may lead to gross errors in predicting column performance. Since the extraction column is the key equipment in sulfolane unit, a non-equilibrium stage model for multicomponent, non-ideal liquid-liquid extraction process^[8] is applied to predict Murphree efficiencies of different components in the column. The results show that the variations of the efficiencies are not negligible because of the change in physical properties and hydrodynamic conditions along the column.
- (4) This software is very convenient to be used. It can be applied to different flowsheet structures, and there are no limits to the maximum numbers of components, process units and streams included in the flowsheet. The software is programmed in C language and can be easily ported to different computer operation systems, such as UNIX and MS-Windows. A friendly interface is developed in Visual Basic especially for PC.

3. Case Studies

As mentioned above, the non-equilibrium stage model can simulate the actual extraction process more accurately than equilibrium stage model. Typical calculated Murphree efficiencies of aromatics along an industrial sieve tray column are shown in Fig. 1. It is evident from the figure that the benzene has highest efficiency and the C₈ and C₉ aromatics have much lower ones because of the difference of their physical properties. In addition, the tray efficiencies of aromatics at the feed stage and lower trays are higher than those of trays at the upper part because of the change of hydrodynamic

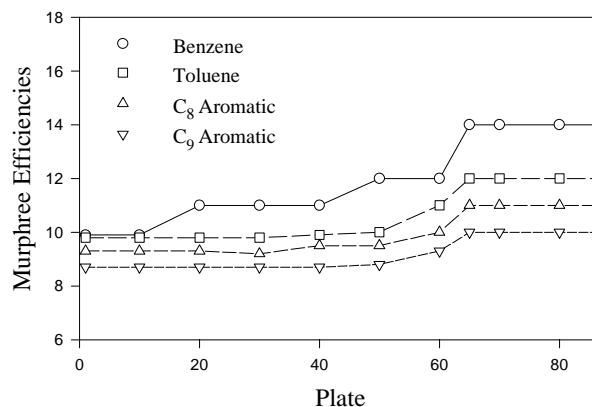


Fig. 1 Calculated Murphree Efficiencies of Aromatics Along the Sieve Tray Column

conditions along the column. Table 1 compares the simulation results of using two models with the operation data. It is clear that using non-equilibrium stage model to simulate the actual extraction process is reasonable, while the assumption of a constant tray efficiency for all components in the column is not justifiable and could cause underdesign, especially for C₈ and C₉ aromatics. Study shows that this assumption in the design of an industrial aromatics plant causes the higher content of C₈ and C₉ aromatics than process specification in the raffinate.

Table 1 Comparison of Simulation Results of Different Models and Operation Data (wt%)

Stream		Benzene	Toluene	C ₈ Aromatics
Raffinate	Operation Data	~0	0.29	1.49
	Simulation 1*	0.0763	0.295	1.49
	Simulation 2*	0.0763	0.163	0.527
Extract	Operation Data	56.8	27.9	15.3
	Simulation 1	52.2	29.2	18.6
	Simulation 2	52.0	29.1	18.8

* Simulation 1 -- Results Using Non-equilibrium Stage Model;

Simulation 2 -- Results Using Equilibrium Stage Model with Constant Efficiency.

The effects of important operation parameters of the extraction column, such as the mass flowrate ratio of solvent to feedstock, the ratio of stripping stream to feedstock, etc., on the recovery ratio and purity of aromatics products could be discussed by this software in detail. Some results are shown in Fig. 2 to Fig. 5. Based on these analyses, the optimal operation conditions could be selected.

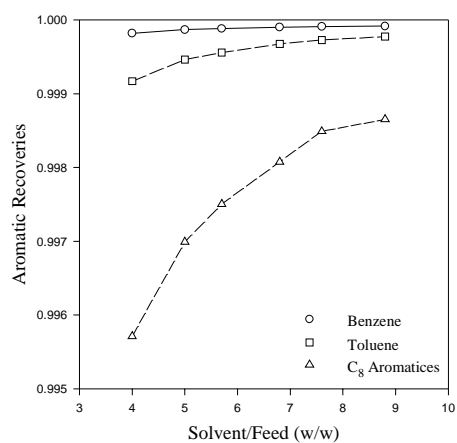


Fig. 2 Effects of Solvent/Feed Ratio on Aromatic Recovery

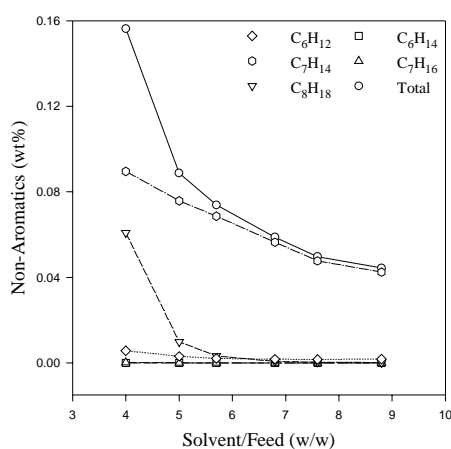


Fig. 3 Effects of Solvent/Feed Ratio on Aromatic Purity

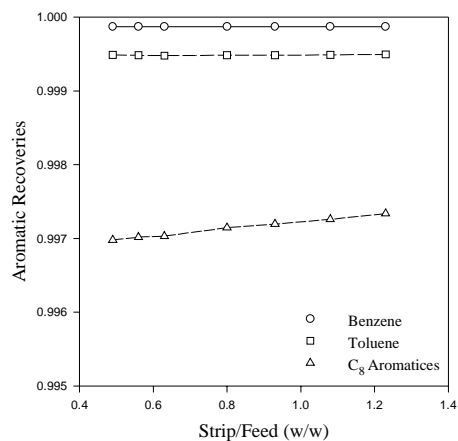


Fig. 4 Effects of Strip/Feed Ratio on Aromatic Recovery

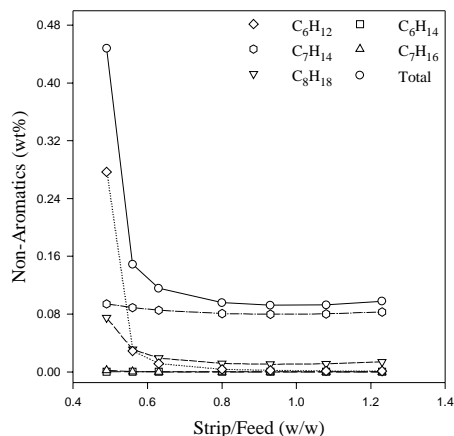


Fig. 5 Effects of Strip/Feed Ratio on Aromatic Purity

4. Conclusion

- 1) The simulation result of this special process flowsheeting system is satisfactory, the software can be applied in the process analysis and design for industrial aromatics plant.
- 2) The application of non-equilibrium stage model can simulate the actual extraction process more accurately than equilibrium stage model.

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