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Simulation of benzene extraction with n-hexane as solvent by Aspen Plus

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Abstract
Benzene is used mainly as an intermediate to make other chemicals. In this study, benzene extraction from binary mixture of benzene and acetonitrile with n-hexane as solvent were simulated at T = 298.15K under atmospheric pressure, respectively. The NRTL modelewas used and suitability of hexane as a solvent were evaluated and selectivity and distribution coefficient were calculated.
The high value of selectivity factors, is reason for be suitable of the solvent for extraction of benzene.

Keywords: Benzene Separation, Acetonitrile, n-hexane, selectivity, NRTL.

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1. Introduction

Benzene is used mainly as an intermediate to make other chemicals, above all ethyl-benzene, isopropyl-benzene, cyclohexane, nitrobenzene, and alkyl benzene. More than half of the entire benzene production is processed into ethyl benzene, a precursor to styrene, which is used to make polymers and plastics like polystyrene.

Ethyne and acetonitrile, catalyzed by organic cobalt dissolved in pure benzene, are used to produce 2-picoline [1]. 2-Picoline is an important pharmaceutical intermediate and organic chemical raw material. In the method, benzene is also one of the byproducts. After 2-picoline and some other byproducts are separated completely from reactant mixtures, there are much mixtures mainly composed of benzene and acetonitrile left, and it is very necessary to separate them for recycle use [2]. In last studies, dimethyl sulfoxide (DMSO) and n-hexane were used as solvent [3]. In this study, n-hexane was chosen as solvent and the separation process was simulated.

Boiling point of benzene and acetonitrile is almost equal, so extraction is one of the best methods of separation.In this simulation, suitability of hexane as a solvent was evaluated and selectivity and distribution coefficient were calculated.

2. Simulation

The feed is a mixture of 70 mole% of benzene and 30 mole% of acetonitrile, with flow rate of 100 kg/hr. The flow diagram for benzene extraction process is shown in fig 1. The extraction column has gotten 3 stages. In first separator (sep1) 0.99 of solvent and in second separator (sep2) 0.99 of acetonitrile were separated.

For this simulation, NRTL activity model was chosen because it was the best model to study phase behavior of Liquid-Liquid Equilibrium for this ternary mixture.

Aspen Plus Simulator was used to calculate the binary interaction parameters, $\mathbf{b_{ij}}$and $\mathbf{b_{ji}}$, in the both equations for the investigated ternary system. The regression method used in the ASPEN simulator was the generalized least squares method based on maximum likelihood principles [2]. The binary interaction is shown in table 1. Mole fraction of components in each stream are presented in table 2.

Table 1.Stream mole fraction.

Stream ID	Benzene	Acetonitrile	N-hexane
S-Benzene	0.930	0.002	0.068
S-Acet-n	0.058	0.804	0.138
Recycle	0.00	0.002	0.998

Table 2.NRTL binary interaction parameters (bij and bji) for the ternary system n-hexane (1) + benzene (2) + acetonitrile (3) .at 298.15 K.

Component i-j	$\mathbf{b_{ij}}$	$\mathbf{b_{ji}}$	$\boldsymbol{\alpha}$	RMDS

1-2	−399.230	762.451	0.3	0.004
1-3	452.227	583.996	0.2	
2-3	263.563	−95.206	0.3	

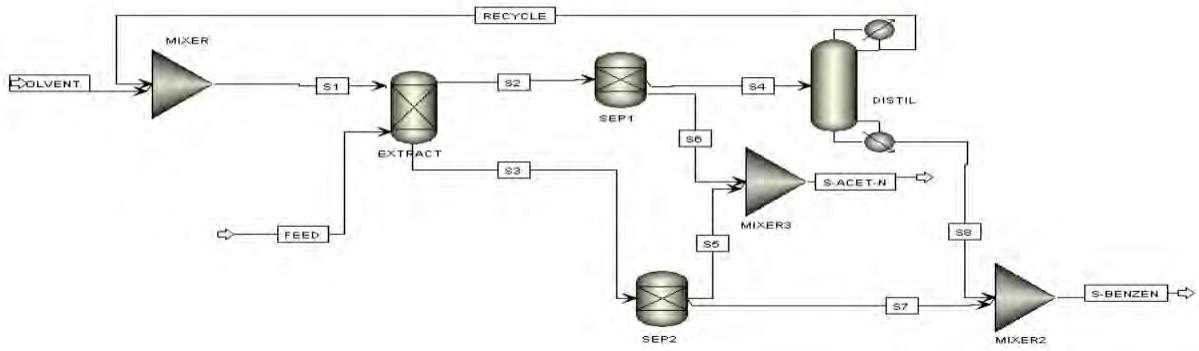

Fig 1.Benzene separation process diagram.

3. Selectivity factor

Selectivity factor is appropriate criteria fr evaluation the ability of the solvent for extraction.

$$D_i = \frac{\text{mole frction in solvent phase}}{\text{mole fraction in Acetonitrile phase}} (1) S = \frac{D_1}{D_2} \quad (2)$$

$D_i$is distribution coefficient for acetonitrile component (i=1), benzene component (i=2).

$$D_1 = \frac{0.027}{0.804} = 0.033 D_2 = \frac{0.064}{0.058} = 1.103 \qquad S = 33.437$$

4. Conclusions

This study simulated the benzene separation process with n-hexane as solvent by Aspen Plus. NRTL activity model was used as thermodynamic equation and NRTL binary interactions, which had been calculated by Aspen Plus simulator, were used in simulation. The selectivity factor for the solvent were calculated and high value of this factor ($S \gg 1$)indicates the suitability of n-hexaneas solvent for extracting benzene from binary mixture of benzene and acetonitrile.

5.Reference

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