

Solvent Screening in Enhanced Distillation Processes on the Total Annual Cost (TAC) Basis

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Abstract

Traditionally the screening of solvents is done by ranking the solvents in the order of the selectivity at infinite dilution. Selectivity at infinite dilution is therefore an important parameter for consideration in the screening of the solvents for an enhanced distillation process including an azeotropic or an extractive distillation process. When solvents are ranked in order of selectivity, the solvent with the highest selectivity is always considered to be the most promising solvent for a given separation. This may indicate that, in economic terms, the use of the solvent with the highest selectivity will always give the lowest total annual cost (TAC) of the enhanced distillation process. How correct is this assertion or how does the order of solvents ranked on the basis of TAC of distillation process vary with the order based on the selectivity of the solvents being considered? This, then, is the focus of this paper. The selectivities of the solvents capable of enhancing the relative volatility of the chosen mixture Ethanol – Water are determined by using the NRTL method for predicting activity coefficients of mixture components. By using the same NRTL (Non-Random Two Liquids) – predicted VLE (Vapor-Liquid Equilibrium) data in both the complete costing and in the determination of the selectivity at infinite dilution, a valid comparison of solvent ranking in terms of the TAC and selectivity at infinite dilution is possible. The obtained results show that for all cases the order of solvents when ranked on the basis of TAC is not the same as when ranked on the basis of selectivity. This means that in general, the matching of selectivity with the TAC for the solvents used in the enhanced distillation process (EDP) of each of the five cases is not perfect.

Keywords: Solvent screening, enhanced distillation, close-boiling mixtures and azeotropic distillation, solvent selectivity.

1. Introduction

The separation azeotropic and close-boiling mixtures by an ordinary distillation process usually results, apart from control problems, in high capital and energy costs. The alternative process of extractive and azeotropic distillation (i.e. an enhanced distillation) has to be used. An enhanced distillation process is generally defined as a distillation in the presence of a substance (solvent) which is relatively nonvolatile compared to the components to be separated [1]. In the presence of the solvent, the relative volatility of the components to be separated increases, thereby making the otherwise difficult separation an easy one and hopefully leading to a reduction in the overall cost of the process. Therefore, at the heart of an enhanced distillation process is the selection of a solvent capable of enhancing the relative volatility of the two key components to be separated.

Traditionally, the screening of such solvents is done by ranking the solvents in the order of their

selectivity at infinite dilution [1]. Selectivity at infinite dilution is therefore an important parameter for consideration in the screening of solvents for an enhanced distillation process. This is usually defined as γ_i/γ_j [1], where γ_i and γ_j are the activity coefficients of components i and j at infinite dilution in the solvent.

Over the years, numerous articles have appeared in the literature on various aspects of the enhanced distillation processes [1-6]. When solvents are ranked in the order of selectivity, the solvent with the highest selectivity is always considered to be the most promising solvent for a give separation.

This may indicate that, in economic terms, the use of the solvents with the highest selectivity will always give the lowest total annual cost (TAC) of the enhanced distillation process (the separation and recovery column taken together). How correct is this assertion or how does the order of the solvents ranked on the basis of total annual cost EDP vary with the order based on the selectivity of the solvents being considered?

In spite of the volume of work that has been done on the screening of the solvents for an enhanced

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distillation process by using selectivity at infinite dilution, the issues raised above are yet to be investigated. This, then, is the focus of this paper. The structure of the paper is as follows: for the separation of the mixture Ethanol/Water by five solvent (1) 1,5-Diamine Pentane; (2) Hexachloro Butadiene; (3) Ethylene Glycol; (4) Glycerol; and (5) Diethylene Triamine, we first determine the optimum solvent feed rate $(S/F)_{opt}$ for use in the optimum design of an enhanced distillation process. The solvents are then ranked in the order of their selectivity at infinite dilution. The TAC of the EDP is calculated for each of the five solvents. The ranking in the order of the solvent selectivity at infinite dilution is then compared with that obtained for the TAC of the EDP for each of the solvents. This is followed by discussion of the results and our conclusions.

2. Determination of the selectivity of the solvents at infinite dilution

Quantitatively, selectivity is defined as the ratio of the relative volatilities of the key components in a mixture, which are to be separated, in the presence of a solvent their relative volatilities before the addition of a solvent [1]. Thus, the selectivity (S_{ij}) can be calculated following equation:

$$S_{ij} = \frac{\alpha_{ijs}}{\alpha_{ij}} \tag{1}$$

where, i and j are key components, s is solvent.

But at low to moderate pressures and temperatures:

$$\alpha_{ij} = \frac{\gamma_i p_i^*}{\gamma_j p_j^*} \tag{2}$$

where p_i^* , p_j^* are the pure component vapor pressures. As the activity coefficients depend on the phase compositions, and the role of the solvent tends to increase with an increase in its concentration, it is common practice to consider the situation of infinite dilution. Then the definition of selectivity at infinite dilution becomes, from equation (2):

$$S_{ij}^{\infty} = \frac{\gamma_i^{\infty}}{\gamma_j^{\infty}} \tag{3}$$

The selectivity of the five solvents capable of enhancing the relative volatility of the chosen mixture Ethanol – Water are determined by using the NRTL method for predicting activity coefficients of mixture components. The results are presented in Table 1.

Table 1. Selectivity at infinite dilution (S^{∞}) for Ethanol – Water mixture

Solvent	$S_{ij}^{\infty} = \frac{\gamma_i^{\infty}}{\gamma_j^{\infty}}$
1-5 Diamine pentane (1)	0.5048
Diethylene Triamine (2)	0.8066
Glycerol (3)	1.0110
Ethylene Glycol (4)	1.4397
Hexachloro butadiene (5)	3.1842

3. Optimum solvent feed rate

For use in the optimum design of an enhanced distillation process, we first determine the optimum solvent feed rate $(S/F)_{opt}$. A fundamental flow sheet for accomplishing an EDP is shown in Fig.1.

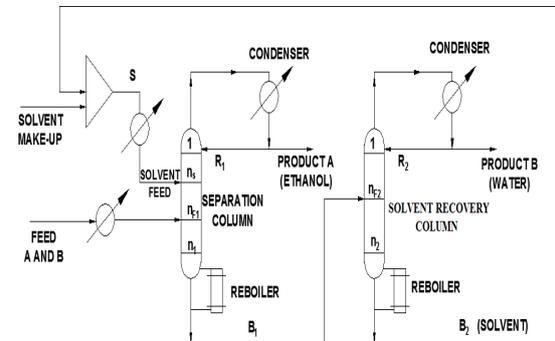


Fig. 1. Typical enhanced distillation process

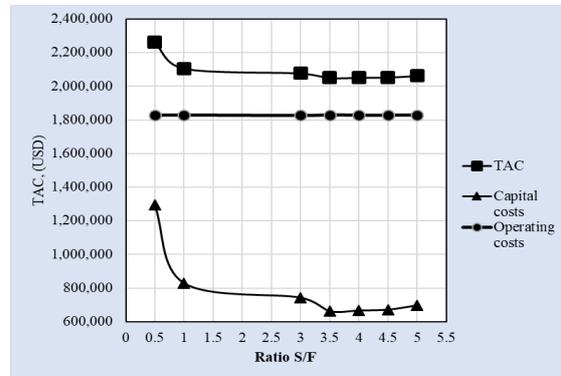


Fig. 2. Optimum solvent rate for enhanced distillation of the mixture Ethanol/Water/Ethylene Glycol

The solvent feed rate is generally a compromise between improved separability with increasing solvent concentration and increasing cost of solvent recovery at increased flow rate. An increase in feed rate increases the relative volatility α_{ij} of the components to be separated, thus decreasing the number of plates required.

Some workers have used a solvent feed rate from about two time [1] to 9 times [3] the feed rate of

the mixture to be separated. We note that these values of optimum solvents rate were arbitrarily picked. In this paper, however, the determination of the optimum solvent feed rate is obtained on the basis of the economic design of the process.

The capital and the operating costs for an EDP are determined as explained later. This is done for the mixture Ethanol – Water with initial ethanol concentration $x_F = 0.885$ mole fraction, and Ethylene Glycol as the solvent. The solvent feed rate S/F is varied from 0.5 to 5.0 kmol/kmol of the feed rate of the key components (Ethanol-Water). The results are given in Table 2 and displayed in Fig.2.

Table 2. The optimum solvent feed rate for Ethanol/Water/Ethylene Glycol enhanced distillation process

S/F	0.5	1	3	3.5
TAC(USD)	2,261,104	2,105,960	2,076,783	2,050,162
S/F	4	4.5	5	
TAC(USD)	2,051,436	2,053,183	2,061,790	

4. Economic evaluation of the enhanced distillation process for the comparison of solvents

The economic evaluations were carried out by using different solvents for separating azeotropic mixture Ethanol-Water: Ethanol/Water/1,5-Diamine Pentane, Ethanol/Water/Hexachloro Butadiene, Ethanol/Water/Glycerol, Ethanol/Water/Diethylene Triamine, Ethanol/Water/EthyleneGlycol. For each case we did a complete design and costing of the process by using Aspen Plus computer programs (version 11). The NRTL method was used to establish the VLE data for the components. By using the same NRTL-predicted VLE data in both the complete costing and in the determination of the selectivity at infinite dilution, a valid comparison of solvent ranking in terms of the TAC and selectivity at infinite dilution is possible.

The TAC is calculated for each solvent rate. We use the TAC formula of Li and Bai (2012) [6]:

$$TAC = \frac{\text{Capital cost}}{\text{Payback period}} + \text{Operating costs}$$

The payback period is considered 3 years. The capital cost includes column shell, tray and heat exchange costs; the operating costs include the reboiler and condenser energy cost. Other costs such as the liquid delivery pumps, pipes, valves are neglected. The optimum solvent rate is taken from the results obtained in section 3 above. The entering feed stream to the enhanced column is taken to be 88% molar composition of Ethanol.

5. Results, discussions, and conclusions

The results of TAC calculation used for the determination of the optimum solvent feed rate for the separation of Ethanol – Water mixture by using the various solvents (1,5-Diamine Pentane, Hexachloro Butadiene, Ethylene Glycol, Glycerol and Diethylene Triamine), are displayed in Fig.2,3,4,5,6. Table 3 shows the ranking of solvent selectivity at infinite dilution with the TAC of the EDP for separation of Ethanol-Water mixture by the five potential solvents.

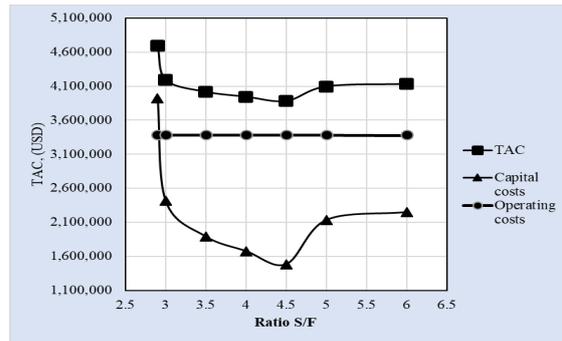


Fig. 3. Optimum solvent rate for enhanced distillation of the mixture - Ethanol/Water/1,5 Diamine Pentane

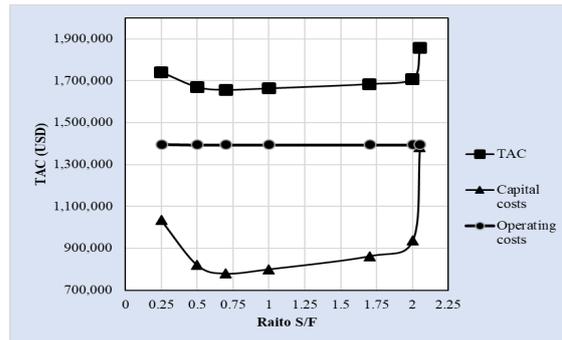


Fig. 4. Optimum solvent rate for enhanced distillation of the mixture - Ethanol/Water/Diethylene Triamine

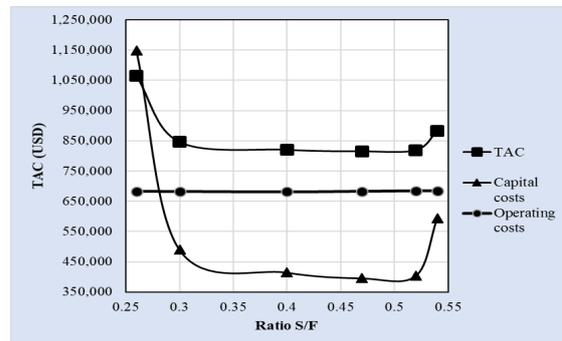


Fig. 5. Optimum solvent rate for enhanced distillation of the mixture - Ethanol/Water/Glycerol

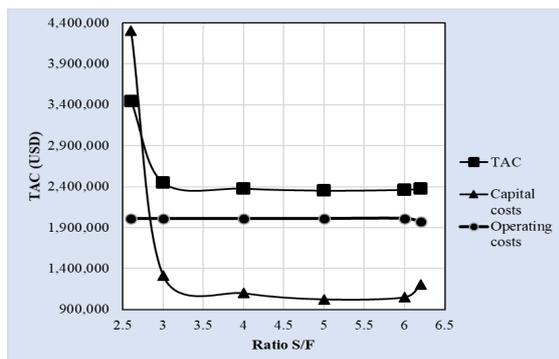


Fig. 6. Optimum solvent rate for enhanced distillation of the mixture - Ethanol/Water/Hexachloro Butadiene

Table 3. Relationship between TAC and selectivity at infinite dilution (S^∞) for Ethanol-Water mixture

Solvent	S^∞	Order	TAC, USDollars	Order
Hexachloro butadiene	3.1842	1	2,229,824	4
Ethylene glycol	1.4397	2	2,001,256	3
Glycerol	1.0110	3	676,695	1
Diethylene triamine	0.8066	4	1,656,335	2
1,5- diamine pentane	0.5048	5	2,272,019	5

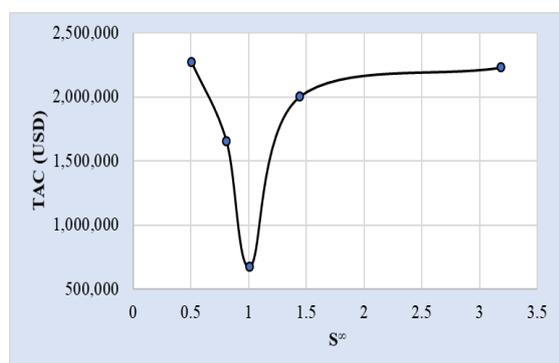


Fig. 7. The effect of solvent selectivity on the total annual cost of an enhanced distillation operation for - Ethanol-Water mixture

The results show that the optimum solvent feed rate is varied in large range (from $S/F = 0.25$ to 5.0). This is not in agreement with values that have been suggested by rules of thumb in the literature [4]. So, to determine the optimum solvent feed rate (S/F)_{opt} for each case, it is necessary to have the curve of TAC as a function of the solvent feed rate (S/F) (see

fig.7). This value is considered appropriate for further analysis and keeps the solvent recovery cost in second column to a minimum.

6. Conclusions

The obtained results show that for all cases the order of solvents when ranked on the basis of TAC is not the same as when ranked on the basis of selectivity. This means that in general, the matching of selectivity with the TAC for the solvents used in the EDP of each of the five cases is not perfect. Based on the results of this work, the following conclusions are made:

- First of all, since the solvent is the core of enhanced distillation, more attention should be paid on the formation of the list of the potential solvents, based on the solvent selectivities at infinite dilution. We observe that selectivity at infinite dilution is a useful tool but not necessarily always accurate in screening solvents for an enhanced distillation process.

- Second, in order to choose the best solvent in economic terms, it is necessary to rank the solvents from the list of potential solvents on the basis of the total annual cost (TAC) (that obtained by design and costing equations by using Aspen plus software). Of course, the smaller the TAC of the EDP, the better the solvent. In other words, when solvents are ranked in the order of increasing TAC, the solvents that are high in the ranking table are the most likely choices for use in the EDP.

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