Extractive Distillation Approach to the Separation of Styrene from Pyrolysis Gasoline Feedstock Coupled with Deep Desulfurization

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Abstract: The separation of mixtures with close boiling points is a critical task in the petrochemical industry, and one such mixture that requires separation is o-xylene/styrene. The STED process is used to separate o-xylene/styrene, which contains a certain amount of organic sulfur in the product due to the limitations of the process. In this study, the process underwent enhancements to attain the effective separation of styrene and accomplish deep desulfurization. A mixture of sulfolane (SUL) and N-methylpyrrolidone (NMP) was selected as the extraction solvent after calculating the UNIFAC group contributions. An orthogonal experiment was conducted to investigate the effects of the solvent/oil ratio, reflux ratio, water addition rate, and solvent ratio on the product. The correspondence between each factor and the indexes examined was determined, enabling the optimization and prediction of the styrene product quality. The final optimized conditions for the extractive distillation column are as follows: solvent/oil ratio of 7, reflux ratio of 4.5, water addition rate of 6000 kg/h, and a solvent ratio of 9:1. Under optimal conditions, the purity of the product was observed to be greater than that of the original process and the sulfur content of the product can be reduced to lower than 10 ppm at the cost of an increase of 12.31% in energy consumption.

Keywords: styrene; o-xylene; organic sulfur; aspen plus

1. Introduction

Styrene represents a significant basic chemical raw material utilized in the synthesis of resins, rubber, and other polymer materials, reaching millions of tons of global annual consumption [1]. Styrene is produced through two methods: the dehydrogenation of aromatic hydrocarbons and recovery from the petroleum refining process [2–6]. Apart from being synthesized through the dehydrogenation of ethylbenzene, styrene can be separated from the pyrolysis gasoline, typically having styrene concentrations ranging from 4% to 6% [7,8]. The increasing demand and high added value of styrene stimulate the development of techniques for styrene recovery from pyrolysis gasoline. Moreover, the efficient recovery of styrene from such sources aligns with contemporary trends towards environmentally sustainable and clean chemical practices.

Pyrolysis gasoline is a byproduct resulting from the process of naphtha cracking. Its primary constituents comprise aromatics, specifically ethylbenzene and xylene, alongside varying quantities of mono-olefins, diolefins, straight-chain alkanes, and cycloalkanes [9]. One considerable challenge in extracting styrene with high purity from pyrolysis gasoline is the separation of styrene and o-xylene, two components that have very close boiling points (145.2 °C vs. 144 °C, respectively) [10–12]. Efficient methods employed for the separation of styrene/o-xylene include extractive distillation, ionic liquid extraction, and adsorption based on porous materials [13–17]. The implementation of ionic liquids and porous materials on a large-scale industrial basis is hindered by their high cost and extreme difficulties in recovery or regeneration [18–23]. Extractive distillation finds the most widely applications in this separation practice [24–26]. Specifically, such process is accomplished by changing the relative volatility of distillation components through the incorporation of auxiliary solvents, such as sulfolane, N-methylpyrrolidone, and N-formylmorpholine [27–29].

Several typical extraction technologies for styrene recovery from cracking gasoline, including the GT-Styrene process [30] and the (Extractive distillation of styrene from pyrolysis gasoline) STED [31] process, have been developed by GTC Technologies (Houston, USA) and Sinopec Petrochemical Scientific Research Institute (Shanghai, China). A general flowchart of the STED process is shown in Figure 1. Previous work focused only on the separation of styrene from pyrolysis gasoline feedstock using different extractants [19,27–29,32]. However, in practice, various products obtained from petrochemical processes often contain a variety of sulfide compounds. Typically, several organosulfides, such as dimethylthiophene, propylthioether, and pentanethiol, are rich in the products of styrene during the extractive distillation process using sulfolane due to the large dissolving affinity of sulfides in the sulfolane solvent. Specially, most difficulties are found in the removal of dimethylthiophene and propylthioether because of their very low relative volatilities. Additionally, the separation of o-xylene/styrene requires 75–80% of the total energy consumption of the entire process [9]. It is crucial to optimize the styrene extractive distillation process for enhanced desulfurization efficiency.
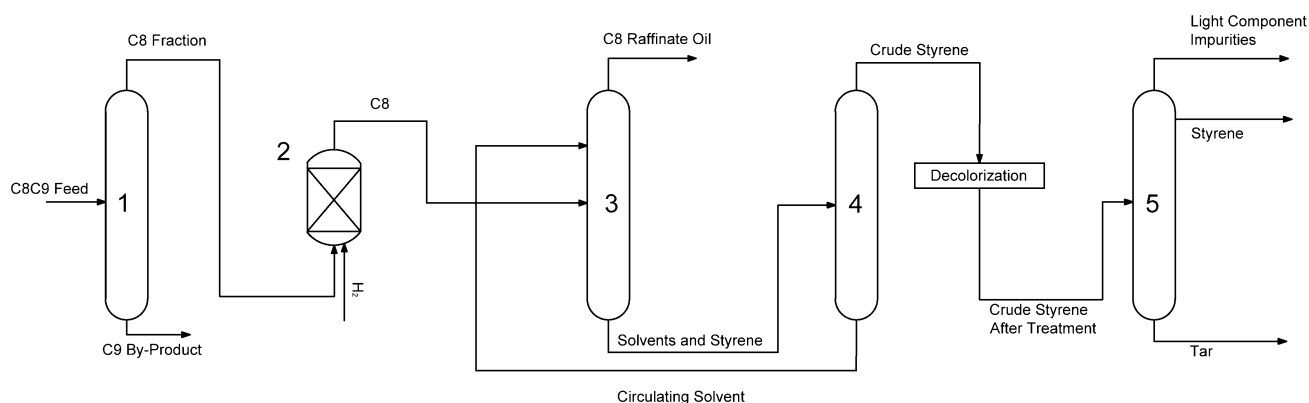

Figure 1. Recovery of styrene from pyrolysis gasoline using the STED process. 1—C8 cutting column, 2—phenylacetylene hydrogenation reactor, 3—extractive distillation column, 4—solvent recovery column, 5—product column.

The present study provides an extractive distillation approach to the separation of styrene from pyrolysis gasoline feedstock coupled with deep desulfurization. The UNIFAC group contribution method was utilized to calculate the activity coefficients and selectivity of alternative extraction solvents and determine the extractant compositions. Process simulations were carried out to evaluate the efficiencies of styrene separation and sulfide removal via the utilization of different extractants. The optimal operating conditions were determined through orthogonal experiments, and the effect of different operating conditions on product quality was evaluated using both extreme difference and variance analyses. In addition, a regression model was developed to predict the quality of the

product under different operating conditions. The present study highlights a practical solution for achieving the efficient recovery of styrene from pyrolysis gasoline along with the deep desulfurization of the product.

2. Methods

2.1. Process Simulation

2.1.1. Calculation of Activity and Selectivity Coefficients

The UNIFAC group contribution method was employed to calculate the activity coefficients of all components, then the activity coefficients were used to determine the selectivity of different extractants towards the target component [33–36]. The selectivity coefficients were used for the preliminary screening of potential desulfurization extractants.

The properties of an extractant molecule are evaluated from the nature of its central atom or group and the substituents attached to this active center. The central atom or group of the extractant molecule typically consists of ligand atoms, such as oxygen, nitrogen, and sulfur, which have a high electronegativity. These ligand atoms can form basic or acidic functional groups. Meanwhile, the central atom or group also contains unshared electron pairs that can interact with other compound molecules. Furthermore, the selectivity, solubility, and stability of each extractant are significantly influenced by the induction, conjugation, hyperconjugation, and spatial site resistance of the substituents connected to the active center atom. From the perspective of the physical and chemical properties, the initial selection of extractants should depend on solubility, selectivity, boiling point, toxicity, price, and thermal and chemical stability and other aspects. The addition of a small amount of water can significantly affect the intermolecular interactions in the separation systems. This is because water readily dissolves in extractants and has a high polarity. Specially, the selectivity of the organic extractant can be largely improved by adding a certain amount of water into the solvent [8,10,12,28].

The component with the highest boiling point in the system is styrene, which is extracted as the heavy key component. The three xylene isomers, styrene, and the organic sulfides have very similar boiling points. Specifically, the differences in boiling points between styrene and 3,4-dimethylthiophene, o-xylene, dipropyl sulfide, and pentanethiol are 0.5 °C, 1.2 °C, 3.5 °C, and 18.7 °C, respectively [2,3]. Thus, the greatest challenge is the separation of 3,4-dimethylthiophene from the styrene product. The polarity of styrene is stronger than that of o-xylene but weaker than that of 3,4-dimethylthiophene. As a result, the non-idealities of the three systems, namely 3,4-dimethylthiophene/styrene, o-xylene/styrene, and dipropyl sulfide/styrene, play a significant role in the selection of an appropriate extractant.
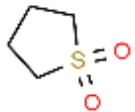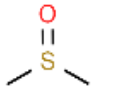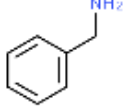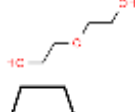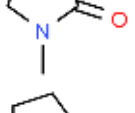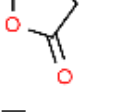
Therefore, a preliminary screening of commonly used extractants for o-xylene/styrene separation and other processes was conducted according to the above analysis. These extractants used in our work have been widely employed in various industrial processes and academic research [27–29]. The structures and properties of all alternative extractants are listed in Table 1. The functional groups of the compounds and the corresponding group volume and surface area parameters are listed in Tables S1 and S2, respectively [33,36–38].

The relative volatilities (α_{ij}) of all components in the system are close to 1, and therefore the selectivity coefficient (S_{ij}) of the extractant can be simplified using Equation (1).

$$S_{ij} = \frac{\alpha_{ijs}}{\alpha_{ij}} = \alpha_{ijs} = \frac{y_i/x_i}{y_j/x_j} = \frac{\gamma_{is}p_i^s}{\gamma_{js}p_j^s} \tag{1}$$

where x is the molar content of component i or j in the liquid phase, y is the molar content of component i or j in the gas phase, γ is the liquid phase activity coefficient of component i or j, and p^s is the saturation vapor pressure of pure component i or j, in mmHg. α is the relative volatility of components i or j. The greater deviation of α from 1 suggests an easier separation of the binary mixture through distillation.

Table 1. Structures of all alternative extractants.

Extractant	Molecular Structure	Ligand Atom	Functional Group	Strength of Polarity	Molecular Weight	Density, $kg \cdot m^{-3}$	Boiling Point, °C	Melting Point, °C	Viscosity, mPa·s	Toxicity
Sulfolane (SUL)		S	S=O	Strong	120.17	1.261	287.1	27.4	10.286	None
Dimethyl sulfoxide (DMSO)		S	S=O	Strong	78.13	1.100	190.7	18.4	1.987	Slight
Benzylamine (BAZ)		N	-NH$_2$	Strong	107.15	0.981	184.5	−30.0	1.599	Moderate
Diethylene glycol (DEG)		O	-O-, -OH	Strong	106.12	1.118	245.0	−10.0	35.700	Slight
N-Methylpyrrolidone (NMP)		N	C=O	Strong	99.13	1.028	204.0	−24.0	1.650	Low
1,4-Butyrolactone (γ-BL)		O	-O-, C=O	Strong	86.09	1.120	204.0	−45.0	1.700	Low
Water	—	O	-OH	Strong	18.02	1.000	100.0	0.0	2.980	None

The activity coefficient (γ_{is}) is calculated for the component using the UNIFAC group contribution method. The saturation vapor pressure, p_i^s, is calculated using the Antoine equation (see Equation (2)). Subsequently, the S_{ij} can be obtained.

$$\log p_i^s = A - \frac{B}{T + C} \tag{2}$$

T is the system temperature, in °C, and A, B, and C are the Antoine equation coefficients.

2.1.2. Construction of the Process Flowchart

The process simulation was carried out using Aspen Plus V11, while the RadFrac model was used for the extraction distillation simulation. Models, including NRTL, UNIFAC, and Wilson equations, are commonly used for the non-ideal systems [39,40]. The simulation results indicate that the UNIFAC model is the most suitable thermodynamic model for the o-xylene/styrene system [41]. The simulation flowchart was established according to a typical industrial process (Figure 2). The composition of each stream is listed in Table S3.
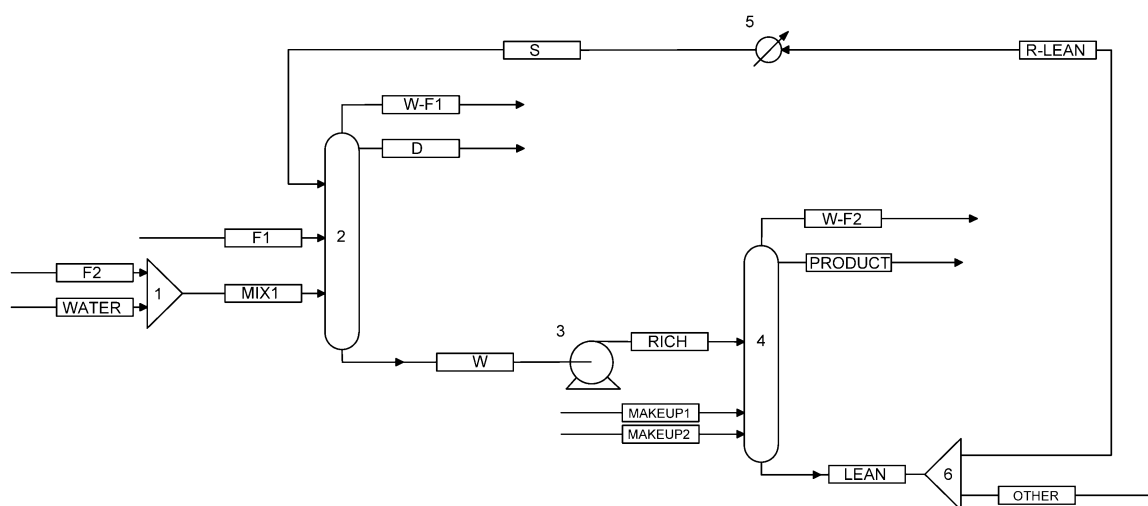

Figure 2. Extractive distillation process for styrene separation from pyrolysis gasoline. 1—Mixer, 2—extractive distillation column, C301, 3—pump, 4—solvent recovery column, C302, 5—heater, 6—spliter.

This process primarily comprises the extractive distillation column (C301), the solvent recovery column (C302), and the heat exchange equipment. The C8 cracked fraction (F1) and lean solvent (S) are introduced into the middle and upper section C301, respectively. Meanwhile, a portion of the crude styrene (F2) is mixed with water and fed into the kettle. The extractant enriched with styrene is directed from the bottom of C301 to C302. Two streams of lean solvent (MAKEUP1, 2) are introduced into the middle section of the C302. The top stream of the column is returned to the column through the condensing section, while a portion is collected as the crude styrene product. The lean solvent at the bottom of the column is recycled to C301.

2.2. Orthogonal Experiment

The orthogonal experiment is employed to obtain the optimal operation conditions [42,43]. The impact of each factor on separation efficiency and energy consumption was identified through the extreme difference and analysis of variance (ANOVA). The ANOVA method is based on the idea of decomposing the total sum of squared deviations into the sum of squared deviations for each different level effect and the sum of squared deviations due to random errors, according to the data structure set. The assumption of the normal distribution is then

used to calculate the statistic F, which is compared with its critical value F_c. This method is used to determine whether the factor will have a significant effect on the results [44–46].

A five-factor, four-level orthogonal experimental design Table L16 (4^5) was utilized, and one factor, the empty column, was reserved for the ANOVA analysis. To achieve the separation of styrene and the removal of organic sulfur, we investigated the following factors: solvent/oil ratio (A), reflux ratio (B), the amount of water added to the column kettle (C), and the extractant ratio of NMP to SUL (D). A and B directly affect the operating conditions and power consumption of the extractive distillation column, and C and D determine the enrichment and purification effect of styrene.

The recovery rate of styrene (y_1, wt%), the weight content of o-xylene in the product (y_2, wt%), the content of organic sulfur in the product (y_3, ppm), and the energy consumption of column C301 (y_4, kW) were considered as the response variables. The factors of the orthogonal experimental design were relatively independent, and no interaction factor was set [47]. The detail information of the factors is listed in Table 2. During the process, if a high separation efficiency, a reduction in organic sulfur content, and the optimization of energy consumption are all desired, the objectives should be ranked in order of importance, as follows: $y_3 > y_1 = y_2 > y_4$.

Table 2. Factors and levels of the orthogonal experiment.

Level	Solent/Oil Ratio	Reflux Ratio	Water Addition Rate	Solent Ratio
	A	*B*	*C*	*D*
1	3	4.5	1500	3:7
2	5	5.0	3000	5:5
3	7	5.5	4500	7:3
4	9	6.0	6000	9:1

2.3. Linear Regression

Multiple linear regression analysis was used to predict one or more response variables (dependent variables) based on a set of predictor variables (independent variables) [48,49].

The equation of multiple linear regression is expressed as $y = w_0 x_0 + w_1 x_1 + \cdots + w_n x_n$, which can be represented in matrix form as $Y = XW$. The dependent variable is represented by Y, while X denotes the independent variable, with the first column of X always set as 1 (the bias column). The coefficients of the independent variable are W, and the independent variable of dimension is N. The objective of multiple linear regression is to identify the W coefficients that are closest to the solution of the linear equation or minimize the sum of squared residuals.

Residual equation is expressed as Equation (3).

$$e_i = y_i - \hat{y}_i \tag{3}$$

The sum of squared residuals can be calculated using Equation (4).

$$Q = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = e_i^T e_i = (y - Xw)^T(y - xw) \tag{4}$$

And

$$e_i \sim N\left(0, \sigma^2\right) \tag{5}$$

$$L = \prod_{i=1}^{M} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i - \hat{y}_i)^2}{2\sigma^2}} \tag{6}$$

$$\ln L = \ln\left(\prod_{i=1}^{M} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i-\hat{y}_i)^2}{2\sigma^2}}\right) = \sum_{i=1}^{m} \ln\left(\prod_{i=1}^{M} \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y_i-\hat{y}_i)^2}{2\sigma^2}}\right)$$
$$= \sum_{i=1}^{m}\left(\ln\left(\frac{1}{\sqrt{2\pi}\sigma}\right) - \frac{(y_i-\hat{y}_i)^2}{2\sigma^2}\right) = \frac{m}{\sqrt{2\pi}\sigma} - -\frac{(y_i-\hat{y}_i)^2}{2\sigma^2} \tag{7}$$

$$max \ln L \Leftrightarrow min \sum_{i=1}^{m} (y_i - \hat{y}_i)^2 \tag{8}$$

$$\frac{\partial Q}{\partial W} = \frac{\partial \frac{1}{2}(Y - XW)^T (Y - XW)}{\partial W} = X^T\left(XW - X^T Y\right) \tag{9}$$

$$\frac{\partial Q}{\partial W} = 0 \Leftrightarrow W = \left(X^T X\right)^{-1} X^T Y \tag{10}$$

W can be obtained from Equations (9) and (10), which leads to the multivariate linear fitting expression. Multivariate linear regression analysis offers an effective way to establish the relationship between a single set of dependent variables and multiple types of independent variables, which helps to minimize the risk of overfitting observed in univariate linear regression analysis. The technique allows for the accurate prediction of the dependent variable when the values of the independent variables are known.

3. Results and Discussion

3.1. Selection of Entrainment Agent for Extractive Distillation

The activity coefficients of the compounds and the selectivity for styrene in different systems are listed in Tables S4 and S5. The selectivity for styrene in different extractants with varying solvent/oil ratios is shown in Figure 3.
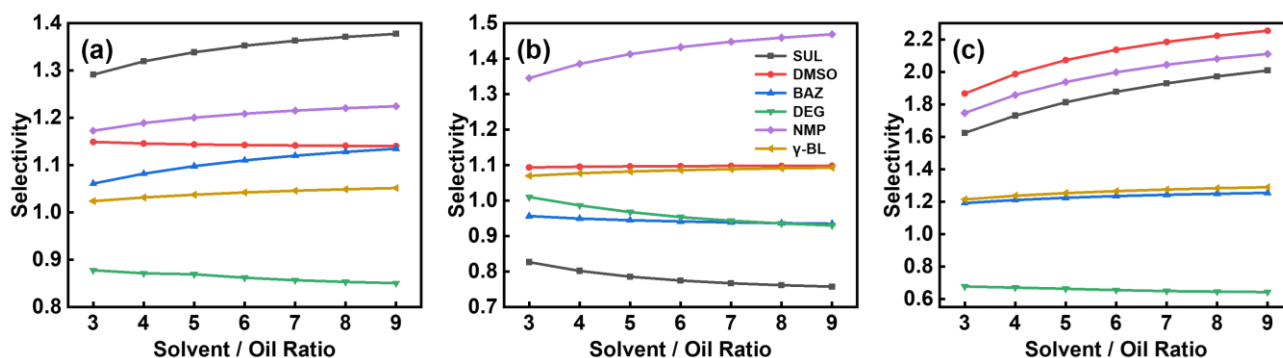

Figure 3. Selectivity of styrene in different extractants over (**a**) o-xylene, (**b**) 3,4-dimethylthiophene, and (**c**) dipropyl sulfide with varying solvent/oil ratios.

SUL exhibits the highest styrene selectivity at the optimal solvent/oil ratio of 3~8 for the o-xylene/styrene system, and NMP takes the second place. Other extractants have limited effects on improving the relative volatility of the system, or even exhibit a higher dissolving affinity to o-xylene than styrene. After achieving the enrichment of styrene, only SUL and NMP need to be considered for other systems that contain sulfides. For the system of 3,4-dimethylthiophene/styrene, only NMP has a high selectivity for styrene. SUL has the lowest selectivity and is deemed as the least favorable extractant for the removal of 3,4-dimethylthiophene from styrene. As for the dipropyl sulfide/styrene system, both NMP and SUL show a higher styrene selectivity compared to other extractants. In summary, NMP was found to be the most effective extractant for the separation of o-xylene/styrene mixture and the removal of sulfides from the styrene product.

3.2. Process Simulation

Using SUL as an extractive entrainment agent, the simulation results and industrial data are summarized in Table 3, indicating the satisfactory simulation accuracy for this sulfide-aromatic systems. To validate the results obtained from the group contribution model, the simulations of extractive distillation were performed using SUL, DMSO, BZA, DEG, NMP, and γ-BL as extractants while maintaining the typical conditions of an industrial plant. Figure 4 shows the obtained simulation results. The styrene recovery rates of different solvents are ranked in the following order: DMSO > SUL > NMP > BAZ > γ-BL > DEG. Correspondingly, the order of the selectivity of styrene over o-xylene is SUL > NMP > DMSO > γ-BL > BZA > DEG. Moreover, the pentanethiol content was reduced to 0 ppm for every extractant case, indicating that the separation of the pentanethiol/styrene system is easy.

Table 3. Simulation results and industrial data.

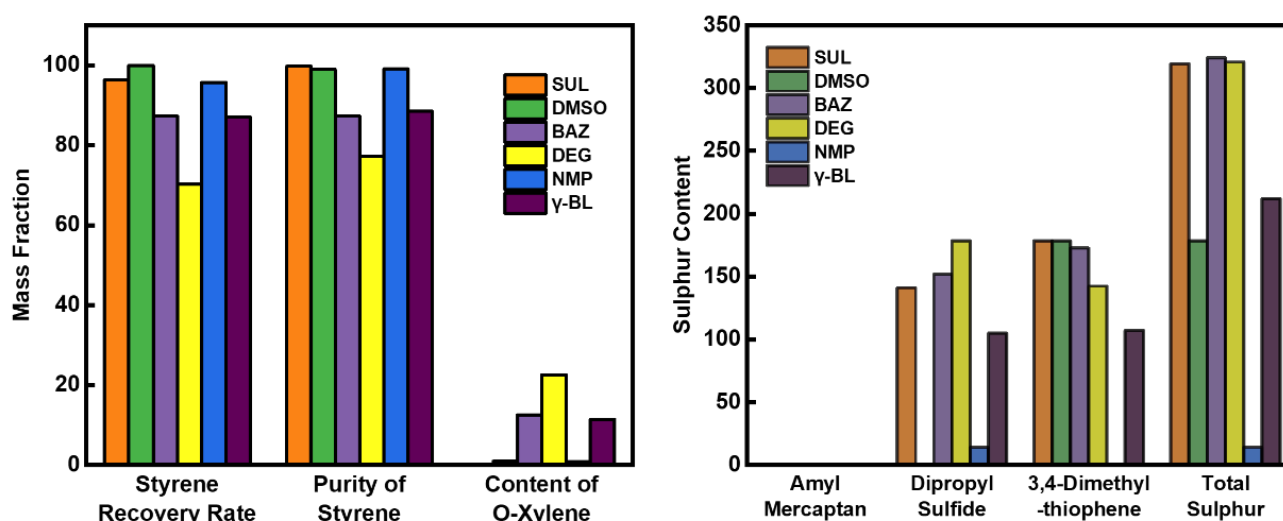| Items	Industrial Data	Simulation Results	Relative Error %
Styrene recovery rate (wt%)	96.43	96.41	0.02
Styrene purity (wt%)	99.78	99.80	0.02
O-Xylene content (wt%)	0.07	0.09	18.60
Organic sulfur content (ppm)	297.469	319.33	6.85

Figure 4. Separation performance of the various extractants under industrial operation conditions.

Among these extractants, only NMP enabled a remarkable reduction in sulfide content. The findings of the process simulation are consistent with the results of the group contribution method. Therefore, in order to achieve a better recovery rate, high product purity, and low sulfur content at the cost of minimal changes in industrial operating conditions, a mixture composed of SUL and NMP was used to achieve the efficient and energy-saving separation of styrene from the o-xylene/styrene mixture with organic sulfides.

3.3. Extreme Difference Analysis of the Orthogonal Experiment

The orthogonal experimental design and the simulation results from Aspen Plus are listed in Table S6. The specific values of the extreme difference analysis are listed in Tables S7–S10. The effect curves for each target under the extreme difference analysis are shown in Figure 5. The order of the primary impact of each factor on y_1 and y_2 is $ACBD$, and the optimal solution is $A_4B_3C_4D_1$. Moreover, the main order of influence on y_3 is $DACB$, and the optimal solution is $A_3B_1C_1D_4$. Additionally, the main order of influence on y_4 is $CBAD$, and the optimal solution is $A_1B_1C_1D_4$. It can be seen from Figure 5a,b that the

factors have entirely contrary effects on y_1 and y_2. Specifically, A is positively correlated with y_1 and negatively correlated with y_2, which promotes the recovery of styrene. The impacts on both y_1 and y_2 can be attributed to the change in the relative volatility of the whole system that resulted from the extractants, which contributes to the increase in styrene recovery rate and the decrease in the content of o-xylene. In an extractive distillation, the reflux ratio can affect the composition of the extraction phase at the plates, leading to the changes in the relative volatility of the system. Under the influence of this aspect, adjusting the reflux ratio is supposed to result in a locally optimal operation. As a result, B_1 was found to be the optimal reflux ratio. From Figure 3 and Table S5, as for the separation of 3,4-dimethylthiophene using SUL as a solvent, it can be observed that a larger solvent/oil ratio does not necessarily mean a higher separation efficiency. In Figure 5d, all factors indicate linear relationships with y_4.
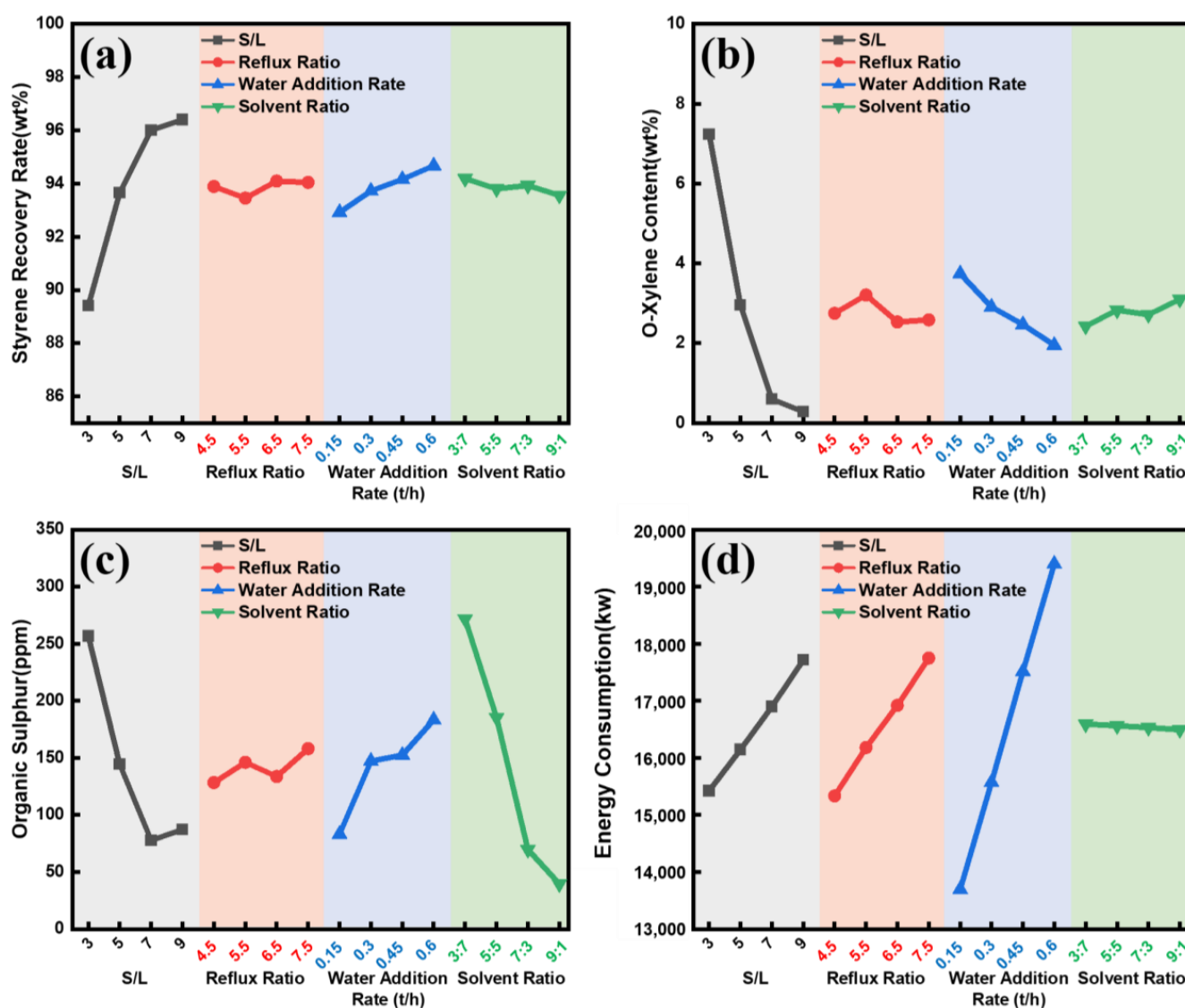

Figure 5. The effects of different factors on the (**a**) styrene recovery rate, (**b**) o-xylene content, (**c**) organic sulfur content, and (**d**) energy consumption.

3.4. ANOVA and Linear Regression

The ANOVA was conducted on y_1, and the results listed in Tables 4 and S11 indicate that the factor A has a significant impact on y_1. The significance analysis results of different factors are listed in Table 5. The results obtained from the ANOVA are consistent with

those of the extreme difference analysis. The negligible error fluctuations indicate that all key factors have been included in the orthogonal experiment. According to the combined analysis of extreme differences and ANOVA, the optimal solution can be determined to be $A_3B_1C_4D_4$. The equation for regression analysis was established by using the data obtained from the simulations. To ensure the accuracy of the model, the validation groups were selected to reflect the range of variation for each factor. Four groups were chosen for the test, while the remaining 12 groups were utilized as the training data.

Table 4. ANOVA results for the styrene recovery rate.

Factors	S-S	DOF	F	Significance
A	123.422	3	86.97815	**
B	1.016	3	0.715997	
C	6.631	3	4.673009	
D	0.811	3	0.571529	
Error	1.419	3		
Total	133.299	15		

** indicates highly significant.

Table 5. Significance analysis of each factor.

	y_1	y_2	y_3	y_4
A	**		**	**
B				**
C				**
D		*		

* indicates relatively significant and ** indicates highly significant.

The regression equation for y_1 is expressed as Equation (11).

$$y_1 = 84.738 + 1.166 * A + 0.220 * B + 0.000 * C - 0.175 * D \tag{11}$$

The regression model analysis on y_1 is listed in Table 6. It indicates that the regression model is statistically significant and has no issue of covariance. Furthermore, the *F*-test ($F = 17.758$, $p = 0.001 < 0.05$) indicates that at least one of *A*, *B*, *C*, or *D* has a significant effect on y_1. The *p*-value analysis confirms the positive effect of *A* on y_1. The linear regression of the other targets can be calculated using Equations (S1)–(S3) and the results are presented in Tables S12–S14. The prediction performance is shown in Figure 6. The predicted results are very close to the industrial values.

Table 6. Linear regression analysis of y_1.

	Non-Standardized Coefficient		t	p	VIF
	B	Standard Error			
Constant	84.738	3.229	26.243	<0.01	-
A	1.166	0.140	8.326	<0.01	1
B	0.220	0.560	0.392	0.703	1
C	0	0	2.037	0.066	1
D	−0.175	0.280	−0.626	0.544	1
R^2		0.871			
F		$F(4,7) = 17.758$, $p = 0.001$			
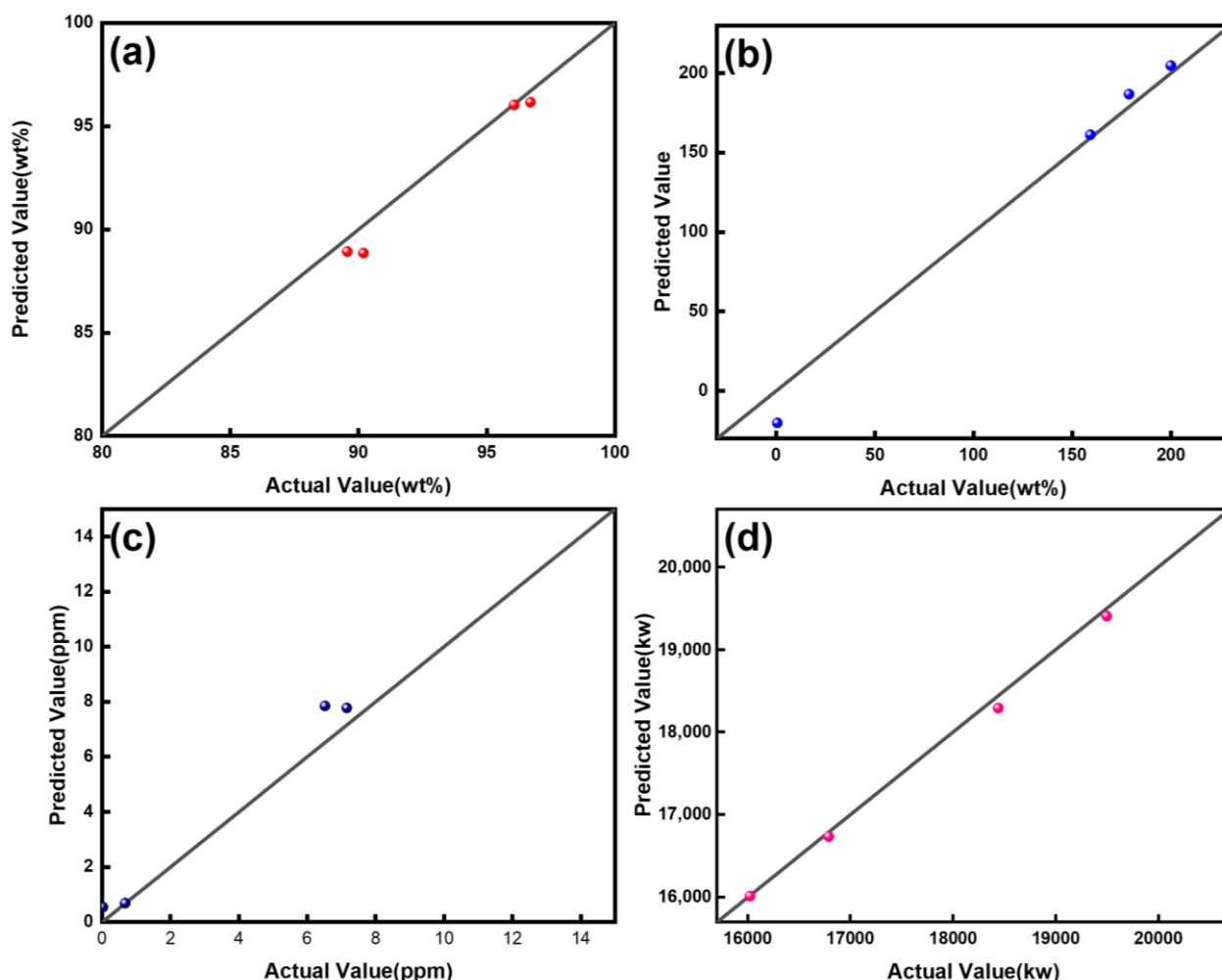
Figure 6. The prediction performances for (**a**) y_1, (**b**) y_2, (**c**) y_3, and (**d**) y_4.

3.5. Simulation Optimization of the Process

The extractive distillation column C301 was optimized under the $A_3B_1C_4D_4$ conditions of solvent/oil ratio of 7, reflux ratio of 4.5, water addition rate of 6000 kg/h, and a solvent ratio of 9:1. The comparison between the original and optimized processes is listed in Table 7. Under optimal conditions, the sulfur content of the product can be reduced to lower than 10 ppm at the cost of an increase of 12.31% in the energy consumption.

Table 7. Comparison of two processes using different solvents.

Items	SUL	Mixed Solvent
Styrene recovery (wt%)	96.41	96.48
Styrene purity (wt%)	99.78	99.84
O-Xylene content (wt%)	0.09	0.02
Organic sulfur content (ppm)	319.33	6.98
Energy consumption (kW)	16,658.6	18,709.09

In the extractive distillation process, the extractant recovery column, C302, plays a crucial role in separating styrene from the extraction solvents. The crude styrene product is obtained as the top distillate and the extractant is recycled at the bottom. Due to the significant difference in boiling point between styrene and the extractant, the effective separation of this mixture is easily achieved. From the simulation results, the purity and water content of the product at the top of the column were considered as the optimization targets. The separation efficiency of C301 has been defined, and the position of the inlet

and outlet flow units of C302 was fixed. As a result, only the influences of the reflux ratio on the contents of styrene, water, and extractant in the product need to be examined (see Figure 7). And the direction of the arrow corresponds to the respective vertical coordinate it is pointing towards. As depicted in Figure 7, using a reflux ratio of 1.5, the purity of styrene is 75.57% and the contents of water and extractant in the product are 1.427% and 22.95%, respectively. As the reflux ratio increases to 3, the purity of styrene substantially increases to 99.20%, and the contents of water and extractant decrease to 0.137% and 0.63%, respectively. As the reflux ratio further increases up to 3.2, the purity of styrene increases up to 99.87%, while the contents of water and extractant decrease to 0.126% and 0, respectively. Therefore, the optimal reflux ratio of extractant recovery column was determined to be 3.2.
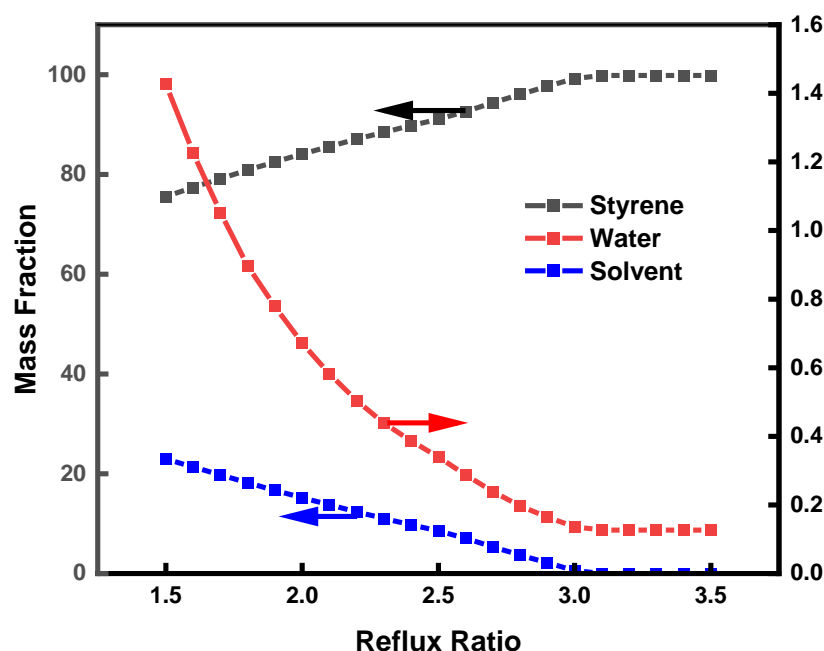
Figure 7. Effect of the reflux ratio on the contents of styrene, water, and extractant in the product. The direction of the arrow corresponds to the respective vertical coordinate it is pointing towards.

4. Conclusions

Aspen Plus V11 was used to investigate styrene products with a high sulfur content produced by a Chinese refinery using STED technology. The UNIFAC group contribution model was used to compute the selectivity coefficients of various extraction solvents for diverse separation systems. The results indicated that NMP could be deemed as the most suitable extractant for the effective separation of styrene from pyrolysis gasoline feedstock coupled with deep desulfurization. However, in order to decrease the fluctuations in operational conditions, a combination of SUL and NMP was used as the extraction solvent. The outcomes of the extreme difference and ANOVA analyses of the orthogonal experiments demonstrate that the key factors that significantly influenced the recovery of styrene, the organic sulfur content, the o-xylene content in the product, and the energy consumption of C301 were the solvent/oil ratio, solvent ratio, solvent/oil ratio, and the amount of added water, respectively. A mathematical regression analysis was carried out on the simulation results to establish the relationship between the impacts of factors on the target. After optimization, the recovery rate of styrene was 96.48%, the purity of styrene in the product was 99.84%, the content of o-xylene in the product was 0.02%, the content of organic sulfur was 6.89 ppm, and the energy consumption was 18,709.09 kW.

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