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

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Table S1. Division of the system component groups.

	Name	Molecular formula	Group division
Compounds in the solution	Octane	C_8H_{18}	$2CH_3,6CH_2$
	1-Octene	C_8H_{16}	$1CH_3,5CH_2,CH_2{=}C$
	Ethylbenzene	C_8H_{10}	$1CH_3,5ACH,1ACCH_3$
	P-xylene	C_8H_{10}	$4ACH,2ACCH_3$
	M-xylene	C_8H_{10}	$4ACH,2ACCH_3$
	O-xylene	C_8H_{10}	$4ACH,2ACCH_3$
	Phenylacetylene	C_8H_6	$5ACH,1CH{\equiv}C$
	Styrene	C_8H_8	$5ACH,1AC,1CH_2{=}CH$
	Cumene	C_9H_{12}	$5ACH,2CH_3,1ACCH$
	n-Nonane	C_9H_{20}	$2CH_3,7CH_2$
	1-Pentanethiol	$C_5H_{12}S$	$1CH_3,3CH_2,1CH_2SH$
	Dipropyl sulfide	$C_6H_{14}S$	$2CH_3,3CH_2,1CH_2S$
	3,4-Dimethylthiophene	C_6H_8S	$2ACCH_3,1CH,1CHS$
Extractant	SUL	$C_4H_8O_2S$	1SULFOLANE
	DMSO	C_2H_6OS	$1Me_2SO$
	BAZ	C_7H_9N	$5ACH,1CH_2NH_2$
	DEG	$C_4H_{10}O_3$	$2OH,3CH_2,1CH_2O$
	NMP	C_5H_9NO	1NMP
	γ-BL	$C_4H_6O_2$	$2CH_2,1CH_2COO$
	Water	H_2O	$1H_2O$

Table S2. Volume and surface area parameters of the component groups.

Group	R_K	Q_K
CH	0.4469	0.228
CH_2	0.6744	0.540
CH_3	0.9011	0.848
CH_2=CH	1.3454	1.176
CH≡C	1.2920	1.088
AC	0.3652	0.120
ACH	0.5313	0.400
ACCH	0.8121	0.348
$ACCH_3$	1.2663	0.968
CH_2COO	1.6764	1.420
CH_2S	1.3863	1.060
CH_2SH	1.6510	1.368
CH_2NH_2	1.3692	1.236
Me_2SO	2.8266	2.827
NMP	2.8266	3.200
SULFOLANE	4.0358	3.200
OH	1.0000	1.200
H_2O	0.9200	1.400

Table S3. Composition of the main streams.

Components	F1 stream	F2 stream
Octane	9.251	0
1-Octene	2.256	0
Ethylbenzene	13.117	0
P-xylene	7.822	0.02
M-xylene	19.103	0.02
O-xylene	10.940	0.07
Phenylacetylene	0.001	0
Styrene	36.552	99.78
Cumene	0.050	0.11
n-Nonane	0.883	0
1-Pentanethiol	0.008	0
Dipropyl sulfide	0.008	0
3,4-Dimethylthiophene	0.008	0

Table S4. Activity coefficients of styrene (STY), o-xylene (OX), and 3,4-dimethylthiophene (3,4-DT) in the different solvents.

S/L	SUL			
	γ_{STY}	γ_{ox}	$\gamma_{3,4\text{-}DT}$	γ_{DS}
3	1.6519	1.8524	1.3435	2.4888
4	1.7709	2.0268	1.3972	2.8432
5	1.8567	2.1551	1.4353	3.1222
6	1.9201	2.2509	1.4635	3.3443
7	1.9679	2.3237	1.4850	3.5232
8	2.0046	2.3797	1.5019	3.6690
9	2.0332	2.4234	1.5155	3.7892
S/L	DMSO			
	γ_{STY}	γ_{ox}	$\gamma_{3,4\text{-}DT}$	γ_{DS}
3	2.1152	3.4387	2.2766	3.6634
4	2.3077	3.8722	2.4883	4.2538
5	2.4484	4.1993	2.6422	4.7081
6	2.5549	4.4544	2.7586	5.0641
7	2.6380	4.6585	2.8493	5.3483
8	2.7046	4.8255	2.9219	5.5792
9	2.7589	4.9646	2.9811	5.7698
S/L	BAZ			
	γ_{STY}	γ_{ox}	$\gamma_{3,4\text{-}DT}$	γ_{DS}
3	1.1422	1.2422	1.0749	1.2623
4	1.1607	1.2873	1.0844	1.3031
5	1.1737	1.3207	1.0910	1.3326
6	1.1832	1.3464	1.0959	1.3547
7	1.1905	1.3667	1.0996	1.3720
8	1.1962	1.3831	1.1025	1.3858
9	1.2009	1.3967	1.1048	1.3971
S/L	DEG			
	γ_{STY}	γ_{ox}	$\gamma_{3,4\text{-}DT}$	γ_{DS}
3	1.0082	1.0073	1.0021	2.7888
4	1.0082	4.4221	4.7656	3.0758
5	5.3356	4.7541	5.0809	3.2810
6	5.6571	4.9974	5.3076	3.4331
7	5.8999	5.1806	5.4758	3.5493
8	6.0865	5.3216	5.6039	3.6402
9	6.2322	5.4322	5.7035	3.7129
S/L	NMP			
	γ_{STY}	γ_{ox}	$\gamma_{3,4\text{-}DT}$	γ_{DS}
3	1.0897	1.1503	1.4429	1.7660
4	1.1012	1.1733	1.5015	1.8978
5	1.1092	1.1896	1.5423	1.9939
6	1.1150	1.2017	1.5722	2.0666
7	1.1195	1.2111	1.5950	2.1233
8	1.1230	1.2185	1.6130	2.1686
9	1.1259	1.2246	1.6274	2.2056

S/L	γ-BL			
	γ_{STY}	γ_{ox}	$\gamma_{3,4\text{-}DT}$	γ_{DS}
3	0.9845	1.2718	1.0364	1.1080
4	0.9828	1.3164	1.0416	1.1269
5	0.9817	1.3496	1.0453	1.1407
6	0.9809	1.3752	1.0481	1.1512
7	0.9803	1.3955	1.0502	1.1594
8	0.9798	1.4121	1.0519	1.1660
9	0.9795	1.4258	1.0533	1.1715

Table S5. Selectivity of each solvent for the systems of o-xylene/styrene, 3,4-dimethylthiophene/styrene, and dipropyl sulfur/styrene.

S/L	O-Xylene/Styrene					
	SUL	**DMSO**	**BAZ**	**DEG**	**NMP**	**γ -BL**
3	1.2911	1.1490	1.0609	0.8776	1.1725	1.0238
4	1.3193	1.1457	1.0819	0.8712	1.1889	1.0315
5	1.3385	1.1437	1.0977	0.8692	1.2003	1.0374
6	1.3524	1.1424	1.1101	0.8617	1.2087	1.0421
7	1.3629	1.1414	1.1199	0.8566	1.2152	1.0458
8	1.3710	1.1407	1.1279	0.8529	1.2203	1.0489
9	1.3775	1.1402	1.1346	0.8503	1.2244	1.0514
S/L	**3,4-Dimethylthiophene/Styrene**					
	SUL	**DMSO**	**BAZ**	**DEG**	**NMP**	**γ -BL**
3	0.8264	1.0935	0.9562	1.0099	1.3454	1.0696
4	0.8016	1.0955	0.9492	0.9864	1.3854	1.0768
5	0.7854	1.0965	0.9445	0.9675	1.4128	1.0819
6	0.7744	1.0970	0.9411	0.9533	1.4326	1.0856
7	0.7667	1.0974	0.9385	0.9430	1.4476	1.0885
8	0.7613	1.0977	0.9364	0.9355	1.4593	1.0908
9	0.7573	1.0979	0.9348	0.9298	1.4687	1.0926
S/L	**Dipropyl Sulfide/Styrene**					
	SUL	**DMSO**	**BAZ**	**DEG**	**NMP**	**γ -BL**
3	1.6236	1.8663	1.1909	0.8763	1.7464	1.2128
4	1.7301	1.9863	1.2098	0.7632	1.8572	1.2356
5	1.8121	2.0722	1.2235	0.6626	1.9372	1.2521
6	1.8769	2.1359	1.2338	0.6540	1.9972	1.2647
7	1.9293	2.1847	1.2419	0.6483	2.0438	1.2745
8	1.9724	2.2230	1.2484	0.6445	2.0809	1.2824
9	2.0083	2.2536	1.2537	0.6420	2.1110	1.2888

Table S6. Orthogonal experimental design and simulation results.

Factor	*A*	*B*	*C*	*D*	Empty	y_1	y_2	y_3	y_4
No.1	3	4.5	1500	3:7	1	88.91	7.75	332.25	11349.46
No.2	3	5	3000	5:5	2	89.12	7.54	337.09	14070.09
No.3	3	5.5	4500	7:3	3	89.51	7.16	199.22	16784.94
No.4	3	6	6000	9:1	4	90.14	6.52	158.43	19490.92
No.5	5	4.5	3000	7:3	4	93.64	2.97	10.46	14012.99
No.6	5	5	1500	9:1	3	91.49	5.20	0.00	12912.50
No.7	5	5.5	6000	3:7	2	95.32	1.22	334.95	19383.34
No.8	5	6	4500	5:5	1	94.16	2.42	232.55	18272.81
No.9	7	4.5	4500	9:1	2	96.34	0.27	0.03	16569.57
No.10	7	5	6000	7:3	1	96.56	0.06	69.08	19309.92
No.11	7	5.5	1500	5:5	4	95.27	1.35	0.52	14507.34
No.12	7	6	3000	3:7	3	95.87	0.72	241.32	17205.51
No.13	9	4.5	6000	5:5	3	96.68	0.01	170.86	19404.08
No.14	9	5	4500	3:7	4	96.65	0.03	178.00	18434.95
No.15	9	5.5	3000	9:1	1	96.28	0.41	0.00	17004.19
No.16	9	6	1500	7:3	2	96.01	0.68	0.00	16019.34

Table S7. Analysis of extreme difference on styrene recovery.

Factor	***A***	***B***	***C***	***D***
k_1	89.42	93.892	92.92	94.188
k_2	93.653	93.455	93.727	93.808
k_3	96.01	94.095	94.165	93.93
k_4	96.405	94.045	94.675	93.563
R_X	6.985	0.64	1.755	0.625
Priority		$A>C>B>D$		
Optimal solution		$A_4B_3C_4D_1$		

Table S8. Analysis of extreme difference on the o-xylene content.

Factor	***A***	***B***	***C***	***D***
k_1	7.242	2.75	3.745	2.43
k_2	2.953	3.208	2.91	2.83
k_3	0.6	2.535	2.47	2.718
k_4	0.282	2.585	1.952	3.1
R_X	6.96	0.673	1.793	0.67
Priority		$D>A>C>B$		
Optimal solution		$A_3B_1C_1D_4$		

Table S9. Analysis of extreme difference on the organic sulfur content.

Factor	*A*	*B*	*C*	*D*
k_1	256.748	128.4	83.192	271.63
k_2	144.49	146.042	147.217	185.255
k_3	77.737	133.672	152.45	69.69
k_4	87.215	158.075	183.33	39.615
R_X	179.011	29.675	100.138	232.015
Priority		$A>C>B>D$		
Optimal solution		$A_4B_3C_4D_1$		

Table S10. Analysis of extreme difference on the energy consumption.

Factor	A	B	C	D
k_1	15423.85	15334.03	13697.16	16593.32
k_2	16145.41	16181.87	15573.2	16563.58
k_3	16898.09	16919.95	17515.57	16531.8
k_4	17715.64	17747.15	19397.07	16494.3
R_X	2291.788	2413.12	5699.905	99.02
Priority	$C>B>A>D$			
Optimal solution	$A_1B_1C_1D_4$			

k_i represents the average purity of styrene at the level i under the same factors. The extreme difference, R_X, is the difference between the maximum and minimum values of the mean product purity under the four factors of A, B, C, and D.

Table S11. ANOVA of y_2, y_3, and y_4.

	Factors	*A*	*B*	*C*	*D*	Error	Total
y_2	*S-S*	123.73	1.13	6.91	0.92	1.54	134.23
	DOF	3.00	3.00	3.00	3.00	3.00	15.00
	F	80.40	0.73	4.49	0.60		
	Significance	**					
y_3	*S-S*	81213.74	2112.04	21208.39	137542.15	16425.29	258501.61
	DOF	3.00	3.00	3.00	3.00	3.00	15.00
	F	4.94	0.13	1.29	8.37		
	Significance				*		
y_4	*S-S*	11626835	12736269	72523485.7	21690.51	41316.09	96949595.93
	DOF	3	3	3	3	3	15
	F	281.41	308.26	1755.33	0.52		
	Significance	**	**	**			

The regression equations for y_2, y_3, and y_4 are presented in **Eq. S1~S3**.

$$y_2 = 11.945 - 1.162 * A - 0.233 * B - 0.000 * C + 0.190 * D \quad (S1)$$

$$y_3 = 360.156 - 28.767 * A + 15.331 * B + 0.020 * C - 81.161 * D \quad (S2)$$

$$y_4 = 1202.705 + 381.402 * A + 1595.489 * B + 1.269 * C - 32.884 * D \quad (S3)$$

Tables S12–S14 list the results of the regression model analysis for y_2, y_3, and y_4, where the R^2 values of the models are greater than 0.8 and the *VIF* values are less than 5. These findings indicate that the regression model is statistically significant and there are no issues with collinearity. The effect of *A* on y_2 will be significantly negative. *C* has a significant positive effect on y_3, while *A* and *D* have a significantly negative effect on y_3. *A*, *B*, and *C* have a significantly positive effect on y_4.

Table S12. Linear regression analysis of y_2

	Non-standardized coefficient		*t*	*p*	*VIF*
	B	Standard error			
Constant	11.945	3.346	3.57	<0.01	-
A	-1.162	0.145	-8.007	<0.01	1
B	-0.233	0.58	-0.402	0.695	1
C	0	0	-2.005	0.07	1
D	0.19	0.29	0.654	0.527	1
R^2	0.862				
F	F (4,7) =17.179, p=0.000				

Table S13. Linear regression analysis of y_3

	Non-standardized coefficient		*t*	*p*	*VIF*
	B	Standard error			
Constant	360.156	156.852	2.296	<0.05	-
A	-28.767	6.8	-4.23	<0.01	1
B	15.331	27.202	0.564	0.584	1
C	0.02	0.009	2.247	<0.05	1
D	-81.161	13.601	-5.967	<0.01	1
R^2	0.843				
F	F (4,7) =14.718, p=0.000				

Table S14. Linear regression analysis of y_4

	Non-standardized coefficient		t	p	VIF
	B	Standard error			
Constant	1202.705	194.263	6.191	<0.01	-
A	381.402	8.422	45.284	<0.01	1
B	1595.489	33.69	47.359	<0.01	1
C	1.269	0.011	113.044	<0.01	1
D	-32.884	16.845	-1.952	0.077	1
R^2	0.999				
F	F (4,7) =4269.090, p=0.000				