ANOMALOUS RESULTS FROM PROCESS SIMULATORS

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A s part of a class assignment in a separations course, students ran an example problem in multicomponent distillation from Holland's textbook[1] on different process simulators. Upon comparison, the results from different simulators were found to differ greatly. Careful examination of both input and output data from the simulation programs revealed no apparent cause for the disparate results.

The simulation results were particularly striking because

- *The major chemical species involved were common industrially important petrochemicals having similar molecular structures.*

- *The processing conditions were very mild, so that nearly ideal conditions should have prevailed in both vapor and liquid phases.*

- *The same thermodynamic package (SRK equation) was used in all cases.*

- *One of the simulators produced a solution in almost perfect agreement with Holland's solution.*

The purpose of this paper is to present the simulation results, to identify the cause of the disparity in these results, and to discuss the implications for separation computations.

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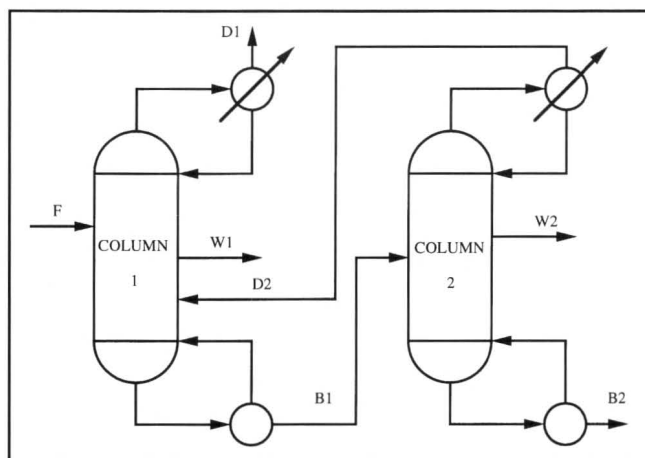
Figure 1. *System of interconnected distillation columns.*

THE DISTILLATION PROBLEM

The problem is taken from Chapter 3 of Holland. The system consists of two interconnected distillation columns, as shown in Figure 1. The feed to the system is defined in Table 1.

Column 1 has 50 trays, a total condenser (stage 1), and a partial reboiler (stage 52). The feed enters on stage 10 as a subcooled liquid at 317.75 K and 270 mmHg. The distillate is withdrawn as a saturated liquid at a rate $D1 = 52$ kmol/h. The sidestream is withdrawn as a liquid from stage 21 at a rate $W1 = 11$ kmol/h. The distillate from column 2 is recycled to stage 45 of column 1. The condenser pressure is 40 mmHg and a linear pressure profile is assumed between stage 2 at 50 mmHg and the reboiler at 270 mmHg. The reflux ratio is 2.5.

The specifications for column 2 are the same as those for column 1 except for the following: the distillate rate is $D_2 = 16$ kmol/h; the sidestream is withdrawn as a liquid from stage 21 at a rate $W2 = 7$ kmol/h; the bottoms from column 1 is fed to column 2 on stage 31; the reboiler

pressure is 250 mmHg rather than 270 mmHg.

RESULTS FROM PROCESS SIMULATORS

The distillation problem was run on Process (Simulation Sciences), Max (Aspen Technology), and Hysim (Hyprotech). To avoid confusion, "Process" will be referred to herein as "Simsci."

Table 2 compares the flow rates of the two major components in each product stream obtained from the simulators with those given by Holland. Note from Table 1 that ethylbenzene and styrene account for nearly 99% of the feed to the system. It can be seen that only Max produced results in agreement with Holland's solution.; the other two simulators

produced results that differ greatly from each other as well as from Holland's solution.

The thermodynamic package used in all three process simulators was the Soave-Redlich-Kwong (SRK) equation of state. Holland's solution was based on ideal solution/ideal gas K-values, with vapor pressure data in the form of Antoine constants. Enthalpy data as well as Antoine constants were obtained from API Project 44.[2]

EFFECT OF MINOR COMPONENTS

Because the minor components were present in such small quantities in the feed, it seemed unlikely that they could be the source of such large discrepancies. To verify this assumption, the distillation problem was rerun with only ethylbenzene and styrene in the feed. The results, given in Table 3, displayed only minor differences from the solutions to the original problem.

EFFECT OF PHYSICAL PROPERTY DATA

Physical property data for the ethylbenzene-styrene system were retrieved from the data banks of the three simulators for comparison. None of the simulators contained binary interaction parameters for this system. Values of pure component parameters are shown in Table 4. With our version of HYSIM we were able to retrieve values of the acentric factor. As can be seen from Table 4, the data for ethylbenzene are in good agreement. For styrene, however, there are significant differences among the simulators, particularly in values of critical temperature and acentric factor.

To determine whether these differences were the cause of the anomalous results from the simulators, the values of T_c, P_c, and ω in Simsci were overriden with the Max values and vice-versa. The results ob-

TABLE 1
Feed Composition

Component	Molar Flow Rate (kmol/h)
Toluene	0.80
Ethylbenzene	51.00
Styrene	47.77
Isopropylbenzene	0.05
1-Methyl-3-ethylbenzene	0.01
α-Methylstyrene	0.13
N-Propylbenzene	0.20
TOTAL	**99.96**

TABLE 2
Results From Process Simulators
(Flow rates in kmol/h)

Stream ID	Component	Holland	Max	Simsci	Hysim
B1	Ethylbenzene	10.11	10.13	19.30	15.22
B1	Styrene	42.53	42.51	33.35	37.42
D1	Ethylbenzene	40.95	41.00	34.05	37.47
D1	Styrene	10.24	10.16	17.11	13.69
W1	Ethylbenzene	5.78	5.82	5.92	5.92
W1	Styrene	5.19	5.16	5.06	5.05
B2	Ethylbenzene	3.02	2.90	8.55	5.63
B2	Styrene	26.60	26.76	21.10	24.03
D2	Ethylbenzene	5.80	5.94	8.19	7.61
D2	Styrene	10.20	10.06	7.81	8.39
W2	Ethylbenzene	1.29	1.29	2.56	1.99
W2	Strene	5.71	5.70	4.44	5.00

TABLE 3
Results from Simulators Excluding Minor Components
(Flow rates in kmol/h)

Stream ID	Component	Max	Simsci	Hysim
B1	Ethylbenzene	10.94	19.73	15.67
B1	Styrene	42.06	33.27	37.33
D1	Ethylbenzene	40.56	33.72	37.20
D1	Styrene	10.21	17.06	13.57
W1	Ethylbenzene	5.82	5.92	5.89
W1	Styrene	5.18	5.08	5.11
B2	Ethylbenzene	3.23	8.82	5.89
B2	Styrene	26.77	21.18	24.11
D2	Ethylbenzene	6.32	8.30	7.76
D2	Styrene	9.68	7.70	8.24
W2	Ethylbenzene	1.39	2.60	2.06
W2	Styrene	5.61	4.40	4.94

TABLE 4
Physical Constants from Different Simulators

	Simsci	Max	Hysim
a) Ethylbenzene			
NBP, K	409.34	409.35	409.27
T_c, K	617.09	617.20	617.09
P_c, mmHg	27071	27047	27055
ω	0.304	0.303	-
b) Styrene			
NBP, K	418.29	418.31	418.27
T_c, K	647.15	636.00	647.54
P_c, mmHg	30020	28802	29986
ω	0.230	0.297	-

tained with these modifications are shown in Tables 5 and 6. They demonstrate conclusively that the anomalous results were indeed due to differences in physical property data for styrene.

While resolving the cause of the differences among the three simulators, the above results raise a number of other questions:

- *Why do the data bases contain such large differences in physical properties for an important compound like styrene?*

- *How sensitive are the simulation results to individual differences in each of the parameters, T_c, P_c, and ω?*

- *Is the observed sensitivity to differences in physical properties typical of separation problems in general, or is it due to some unique aspect of the ethylbenzene-styrene distillation?*

- *To what extent are the observed results due to the choice of thermodynamic package?*

- *Which of the solutions, if any, is the correct solution to the distillation problem?*

These issues are addressed in the remainder of this paper.

PHYSICAL PROPERTIES OF STYRENE

A readily available source (Reid, *et al.*[3]) lists the following properties for styrene:

- Vapor pressures (Antoine equation)

$$\ln\left(P^{sat}\right) = A - B/(T + C)$$

where

$\quad$ A $\quad$ = 16.0193

$\quad$ B $\quad$ = 3328.57

$\quad$ C $\quad$ = -63.72

$\quad$ P^{sat} = vapor pressure in mmHg

$\quad$ T $\quad$ = temperature in K (305 K < T < 460 K)

- Critical temperature $\quad$ T_c = 647 K

- Critical pressure $\quad$ P_c = 29944 mmHg

- Acentric factor $\quad$ ω = 0.257

The critical temperature and pressure reported by Reid, *et al.*, are in general agreement with the values used by Simsci and Hysim., but their reported acentric factor is inconsistent with their reported vapor pressure and critical properties. An acentric factor consistent with the rest of their reported data is

$$\omega = 0.23, \quad \left(\omega = -\log_{10}\left(P_r^{sat}\right)_{Tr=0.7} - 1.0\right)$$

which is also in good agreement with the value retrieved from the Simsci database.

Checking the computerized database of the Thermodynamics Research Center (TRC) at Texas A&M University[4] revealed that there are no measured values for the critical properties of styrene. Hence, all the values of T_c and P_c in the literature and the simulator databases are estimated. The lack of critical data is apparently due to the strong tendency of styrene to polymerize, especially at elevated temperatures.[5] (This is the reason for the vacuum distillation.) Since the acentric factor is determined from vapor pressure and critical point data, the large discrepancy in acentric factor values used by the different process simulators is understandable.

There is good agreement between the vapor pressure values of styrene reported by Reid, *et al.*, and the ones reported by TRC in the temperature range of 305 K to 460 K—they agree within ±0.5%. Above 460 K, there are no reported vapor pressure measurements for styrene. Since 460 K corresponds to a reduced temperature greater than 0.7, the vapor pressure value used to determine the acentric factor should be accurate (no extrapolation of vapor pressure measurements involved). In this case, the sources of error in the calculation of ω are the uncertainty in the estimated value for the critical temperature and the error in the extrapolation of the experimental vapor

TABLE 5
Comparison of Original Max Solution and Simsci Solution with Max Parameters
(Flow rates in kmol/h)

Stream ID	Component	Original Solution from Max	Simsci Solution with Max T_c, P_c, ω
B1	Ethylbenzene	10.13	10.21
B1	Styrene	42.51	42.43
D1	Ethylbenzene	41.00	41.00
D1	Styrene	10.16	10.15
W1	Ethylbenzene	5.82	5.82
W1	Styrene	5.16	5.16
B2	Ethylbenzene	2.90	2.93
B2	Styrene	26.76	26.73
D2	Ethylbenzene	5.94	5.98
D2	Styrene	10.06	10.02
W2	Ethylbenzene	1.29	1.30
W2	Styrene	5.60	5.69

TABLE 6
Comparison of Original Simsci solution and Max solution with Simsci Parameters
(Flow rates in kmol/h)

Stream ID	Component	Original Solution from Simsci	Max Solution with Simsci T_c, P_c, ω
B1	Ethylbenzene	19.30	19.08
B1	Styrene	33.35	33.56
D1	Ethylbenzene	34.05	34.15
D1	Styrene	17.11	17.01
W1	Ethylbenzene	5.92	5.92
W1	Styrene	5.06	5.06
B2	Ethylbenzene	8.55	8.41
B2	Styrene	21.10	21.24
D2	Ethylbenzene	8.19	8.15
D2	Styrene	7.81	7.85
W2	Ethylbenzene	2.56	2.53
W2	Styrene	4.44	4.47

TABLE 7
Simulation Solutions with Simsci
Parameters and Two Different Critical Temperatures
for Styrene
(Flow rates in kmol/h)

Stream ID	Component	Solution with $T_c = 647.15\ K$	Solution with $T_c = 636.0\ K$
B1	Ethylbenzene	19.08	30.45
B1	Styrene	33.56	22.19
D1	Ethylbenzene	34.15	23.29
D1	Styrene	17.01	27.87
W1	Ethylbenzene	5.92	5.85
W1	Styrene	5.06	5.12
B2	Ethylbenzene	8.41	17.75
B2	Styrene	21.24	11.89
D2	Ethylbenzene	8.15	8.59
D2	Styrene	7.85	7.41
W2	Ethylbenzene	2.53	4.11
W2	Styrene	4.47	2.89

TABLE 8
Simulation Solutions with Simsci Parameters and Two
Different Critical Pressures for Styrene
(Flow rates in kmol/h)

Stream ID	Component	Solution with $P_c = 30020\ mmHg$	Solution with $P_c = 28802\ mmHg$
B1	Ethylbenzene	19.08	16.86
B1	Styrene	33.56	35.78
D1	Ethylbenzene	34.15	36.04
D1	Styrene	17.01	15.12
W1	Ethylbenzene	5.92	5.96
W1	Styrene	5.06	5.01
B2	Ethylbenzene	8.41	6.78
B2	Styrene	21.24	22.87
D2	Ethylbenzene	8.15	7.86
D2	Styrene	7.85	8.14
W2	Ethylbenzene	2.53	2.22
W2	Styrene	4.47	4.77

TABLE 9
Simulation Solutions with Simsci
Parameters and Two Different Acentric Factors for Styrene
(Flow rates in kmol/h)

Stream ID	Component	Solution with $\omega = 0.230$	Solution with $\omega = 0.297$
B1	Ethylbenzene	19.08	!.3E-03
B1	Styrene	33.56	52.61
D1	Ethylbenzene	34.15	47.65
D1	Styrene	17.01	3.51
W1	Ethylbenzene	5.92	3.33
W1	Styrene	5.06	7.60
B2	Ethylbenzene	8.41	3.9E-05
B2	Styrene	21.24	29.70
D2	Ethylbenzene	8.15	1.1E-3
D2	Styrene	7.85	15.95
W2	Ethylbenzene	2.53	1.42E-04
W2	Styrene	4.47	6.95

pressure to obtain a value for the critical pressure.

A value of 418.3 K for the normal boiling point of styrene was used to estimate its critical temperature. Three different methods were used: Lydersen's method,[6] Ambrose's method,[3] and the Joback modification of Lydersen's method.[3] The estimated critical temperatures were 635 K, 635 K, and 639K, respectively. The value of 635 K is in good agreement with that of Max (636 K), but it does not agree with the Simsci and Hysim value (647 K).

The acentric factor for styrene was calculated using the vapor pressure equation from Reid, *et al.*, the vapor pressure data from TRC, and a critical temperature of 636 K. Critical pressure was obtained by extrapolation of the vapor pressure data to the critical temperature. The vapor pressure equation from Reid, *et al.*, produced a critical pressure value of 26983 mmHg and an acentric factor of 0.26, while the vapor pressure equation from TRC yielded a critical pressure of 28043 mmHg and an acentric factor of 0.28. The differences are due to the error in the extrapolation of the vapor pressure to obtain the critical pressure. A difference in critical pressure of 3.8% produced a difference of 7% in the acentric factor. The critical pressure and acentric factor obtained with the TRC vapor pressure equation are in relatively good agreement with the values used by Max (P_c = 28802 mmHg and ω = 0.297). Using a critical pressure of 28802 mmHg in the calculation of the acentric factor produced a value of ω = 0.30 with both sets of vapor pressure data.

To summarize, values of T_c, P_c, and ω reported in the literature for styrene are in general agreement with the values in the Simsci and Hysim data banks. However, standard estimation procedures yield values that are consistent with those in the Max data bank.

SENSITIVITY OF SOLUTION TO CHANGES IN T_C, P_C, AND ω

In order to determine the effect of each individual parameter on the solution, simulation runs were made using Simsci parameters except that for styrene, Max values were substituted for either T_c, P_c, or ω. Results of these simulations (which were run using Max) are given in Tables 7, 8, and 9. As can be seen, each parameter had a significant effect on the solution, but T_c and ω had the greatest impact. Interestingly, the effects of T_c and ω are in opposite directions, so that the individual effects are greater than the combined effect of both parameters. The relative changes in parameter values for these runs were, from Table 4b, 1.7% for T_c, 4% for P_c, and 29% for ω.

Additional runs were made in which the styrene acentric factor was varied from 0.230 to 0.275. Simsci values were used for all other parameters. The effect of ω on the bottoms composition from column 1 is shown in Table 10. (The slight discrepancy between the data in Tables 9 and 10 is

TABLE 10
Effect of Styrene Accentric Factor on Separation

ω	% Styrene in B1	ω	% Styrene in B1
0.230	62.83	0.265	83.28
0.245	70.60	0.270	87.36
0.250	75.50	0.275	91.50
0.260	79.81		

due to the fact that the former were obtained from runs on Max and the latter from runs on Simsci.

The effects of the parameters on relative volatility in column 1 are shown in Table 11. (The values for column 2 were similar.) These data were generated using Max with various combinations of the Max and Simsci parameter values as indicated in Table 11. The first two columns of the table give the volatility profiles obtained with all Simsci parameters and all Max parameters, respectively. The volatilities for the two cases are nearly identical at the bottom, but differ significantly over most of the column. Changing individual parameters dramatically alters the volatility as shown in the last four columns of the table. Within the ranges of parameters considered, the data display an apparent reversal in the volatilities of the two components (column 6) and an apparent azeotrope (column 4). Obviously, such differences in relative volatility will greatly affect the separation achieved in the simulations.

COMPARISON WITH OTHER BINARY SYSTEMS

Ethylbenzene and styrene constitute a narrow boiling system with a difference in normal boiling points of 9 K. Since the relative volatility is close to unity, differences in K-values due to differences in T_c, P_c, or ω can have a large effect on the calculated solution.

By the same reasoning, smaller effects would be expected for systems with wider boiling ranges. Calculations were made for the toluene-styrene system (normal boiling point difference of 35 K) and the benzene-styrene system (normal boiling point difference of 65 K) for comparison with the ethylbenzene-styrene system. A modified system consisting of a single column with 20 internal trays, a total condenser and partial reboiler was used. Operating conditions were the same as in Column 1 of the original problem. Feed rate, side-draw rate, and reflux ratio were unchanged. Feed entered on stage 8 (condenser = stage 1) as a subcooled liquid at 317.75 K and 270 mmHg. The bottoms flow rate was specified at 60 kg mole/h. Simulations were run on Simsci using Simsci parameters except for the styrene acentric factor, which was varied from 0.20 to 0.32. The results, shown in Table 12, confirm the expected trend with width of boiling range.

COMPARISON WITH
OTHER THERMODYNAMIC PACKAGES

In order to determine the sensitivity of the results to the choice of thermodynamic routine, runs were made with a number of thermodynamic packages other than the SRK equation.

▶ *Generalized Cubic Equations of State* • The use of other cubic equations, such as Peng-Robinson, had very little effect on the results, as would be expected.

▶ *Ideal Thermodynamic Package* • The assumptions of

ideal gas behavior in the vapor phase and ideal solution behavior in the liquid phase should provide a good approximation for the system under consideration. As previously mentioned, Holland's solution is based on these assumptions. The only property data needed to obtain a solution are then pure component vapor and liquid enthalpies and vapor pressures. (In Max, however, critical temperature is used to estimate latent heat of vaporization, which in turn is used to calculate liquid enthalpy.)

Solutions for the original seven-component system obtained using Max and Simsci are compared with Holland's solution in Table 13. The three solutions are in reasonably good agreement. However, the Max solution still agrees significantly better with Holland's results than does the Simsci solution.

▶ *UNIFAC Thermodynamic Package* • The UNIFAC thermodynamic package in Max uses the generalized Redlich-Kwong equation of state for the vapor phase and the UNIFAC group contribution method for liquid-phase activity coefficients. An activity coefficient method would normally not be used in the present application since the liquid phase behavior should be nearly ideal. However, its use permits the separation of vapor-phase and liquid-phase effects of T_c and P_c. Vapor fugacities are computed with the Redlich-

TABLE 11
Effect of T_c, P_c, and ω on Relative Volatility ($K_{EB}/K_{styrene}$) in Column 1

(S = Simsci value, M = Max value)

Stage	$T_c = S$ $P_c = S$ $\omega = S$	$T_c = M$ $P_c = M$ $\omega = M$	$T_c = S$ $P_c = S$ $\omega = M$	$T_c = M$ $P_c = M$ $\omega = S$	$T_c = S$ $P_c = M$ $\omega = M$	$T_c = M$ $P_c = S$ $\omega = S$
1	1.17	1.42	1.79	0.95	1.85	0.91
13	1.19	1.38	1.69	0.98	1.76	0.94
26	1.20	1.36	1.67	0.998	1.71	0.96
39	1.20	1.34	1.64	1.01	1.68	0.97
52	1.32	1.34	1.61	1.02	1.65	0.97

TABLE 12
Effect of Acentric Factor in Systems with Different Boiling Ranges

(Flow rates in kmol/h)

ω	% Styrene in Bottoms for Benzene-Styrene System $\Delta T_b = 65\ K$	% Styrene in Bottoms for Toluene-Styrene System $\Delta T_b = 35\ K$	% Styrene in Bottoms for Ethylbenzene-Styrene System $\Delta T_b = 9\ K$
0.20	73.92	72.10	48.60
0.23	74.04	72.84	55.20
0.26	74.14	73.26	61.20
0.28	74.19	73.47	64.40
0.32	74.28	73.81	69.60

Kwong equation, which uses T_c and P_c, while the liquid phase calculations using UNIFAC do not involve T_c and P_c. (The Poynting correction factor involves critical parameters since the Rackett equation is used to calculate liquid density. However, this factor is essentially unity at conditions in the distillation system.)

Results obtained for the original seven-component system using Max with both Max and Simsci parameters are shown in Table 14. The two sets of values are nearly identical, demonstrating that effects of T_c and P_c in the simulations using the SRK equation are confined to the liquid phase in the present application. This result is logi-cal since at the very low pressures in the distillation system, the vapor-phase fugacity coefficients should be close to unity and insensitive to errors in critical parameters.

WHICH SOLUTION IS CORRECT?

The results presented above suggest that of the original solutions generated by the three simulators, the solution generated by Max is the correct one. The reasons are:

- *The critical data for styrene in the Max data bank are consistent with the Lydersen and Ambrose correlations, while those in the Simsci and Hysim data banks are not.*

- *The solutions generated by Max using the SRK equation of state and ideal thermodynamics are consistent, while those generated by Simsci (and presumably Hysim as well) are not. Since both thermodynamic packages should be applicable to the distillation system, the solutions should be consistent.*

- *The solution generated by Max is consistent with Holland's solution.*

CONCLUSIONS

The results presented above demonstrate that errors in pure component parameters can have a surprisingly large effect on separation calculations for narrow-boiling mixtures. Therefore, the values of these parameters in the simulator data banks should be checked for possible errors when working with these mixtures.

In the present case, comparison with published data would probably not have disclosed the problem since the published data for styrene critical properties agree with the Simsci and Hysim values. Nevertheless, this should be done. (In an unrelated application, for example, we found in this manner an error in a specific heat in a simulator data bank that caused an incorrect heat exchanger design.) In addition, the data should be checked for consistency with property estimation techniques; large discrepancies may indicate a problem with the data and should be cause for concern.

As recently pointed out by Kister,[7] there is a good deal more involved in process simulation than simply typing in data and obtaining a converged solution. Students need to learn to subject the results obtained from simulators to the same kind of rigorous scrutiny as any other engineering calculation. Inclusion in the curriculum of examples such as the one presented here can help make this point more forcefully than any amount of cautionary lecturing by instructors.

TABLE 13
Comparison of Solutions Obtained Using
Ideal Thermodynamic Package
(Flow rates in kmol/h)

Stream ID	Major Component	Max Solution	Simsci Solution	Holland's Solution
B1	Ethylbenzene	9.86	8.49	10.11
B1	Styrene	42.78	44.15	42.53
D1	Ethylbenzene	41.06	41.90	40.95
D1	Styrene	10.10	9.26	10.24
W1	Ethylbenzene	5.78	5.73	5.78
W1	Styrene	5.19	5.24	5.19
B2	Ethylbenzene	2.91	2.35	3.02
B2	Styrene	26.75	27.30	26.62
D2	Ethylbenzene	5.70	5.07	5.80
D2	Styrene	10.30	10.92	10.20
W2	Ethylbenzene	1.25	1.06	1.29
W2	Styrene	5.73	5.92	5.71

TABLE 14
Comparison of Solutions Obtained Using
UNIFAC Thermodynamic Package in Max
(Flow rates in kmol/h)

Stream ID	Major Component	Solution with Max Parameters	Solution with Simsci Parameters
B1	Ethylbenzene	9.72	9.90
B1	Styrene	42.92	42.74
D1	Ethylbenzene	41.05	41.03
D1	Styrene	10.11	10.12
W1	Ethylbenzene	5.76	5.78
W1	Styrene	5.21	5.19
B2	Ethylbenzene	2.96	2.93
B2	Styrene	26.70	26.73
D2	Ethylbenzene	5.52	5.72
D2	Styrene	10.48	10.28
W2	Ethylbenzene	1.23	1.26
W2	Styrene	5.75	5.73

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