

# BTX제조공정의 모사연구

## Simulation of Benzene-Toluene-Xylene Plant

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### Abstract

This paper deals with modeling and simulation of an industrial benzene-toluene-xylene plant. Because the fractionation unit of benzene-toluene-xylene plant has a narrow range of boiling point and doesn't have any sidecut and side reboiler, we employed boiling point estimation method in the modeling and simulation of the plant. Soave-Redlich-Kwong equation was used in the computation of thermodynamical properties. We solved resulting nonlinear equations by using Newton-Raphson method which is known to show fast convergence. Results of simulations showed good agreement with actual plant operation data.

## 1. Introduction

Automated operations of chemical plants require a lot of up-to-date computer hardwares as well as application softwares. The main duties of application softwares are to perform data handling, optimization of plant operation and advanced controls of related processes. Most of these functions are based on the modeling and simulation of the plant. Recently rapid development of digital computer technology has made it possible to implement more sophisticated simulation techniques in the operation of chemical plants. The purpose of this paper is to demonstrate how to simulate actual chemical plants and how the simulation results can be utilized

in the plant operation.

A benzene-toluene-xylene(BTX) plant consists of hydro-treating unit, extraction unit, fractionation unit and hydro-dealkylation unit. Among these four units, fractionation unit is the major unit and the present work aims at modeling and simulation of the fractionation unit. The fractionation unit mainly consists of three distillation columns and so most of the present work concerns modeling and simulation of distillation processes.

Various methods such as BP, SR and SC have been developed for modeling of distillation processes and each method has proved good performance at specific process[2]. Some of these methods are utilized commercially but

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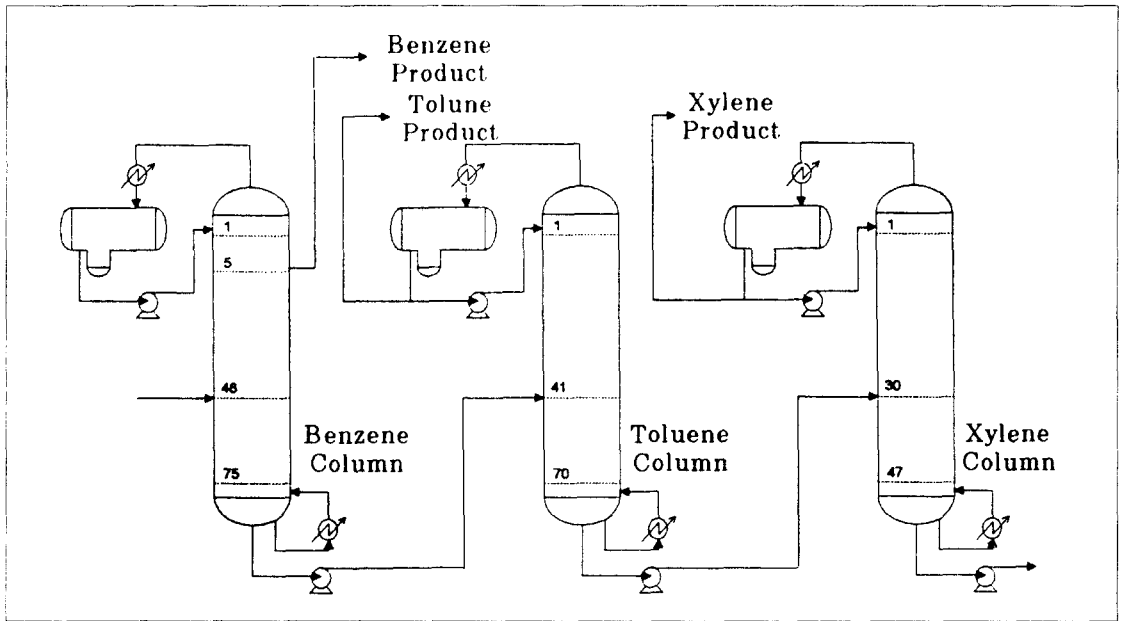
usefulness of those methods depends on the characteristics of the processes employed. Modeling of the BTX plant requires accurate thermodynamical properties of each chemical compounds involved and knowledge of operational constraints. In the present work modifications of the existing method were performed by employing suitable thermodynamical relationships and various operational constraints.

The purpose of modeling and simulation is to develop on-line optimal operation system for BTX plant. The fractionation unit considered in the present work consists of three distillation columns, each of which has 75, 70, and 55 trays respectively. Benzene, toluene and xylene are obtained as top products of each column. Fig.1 shows flow diagram of the fractionation unit.

(Table 1) Feed Composition of BTX-Plant

Component \ Column	Benzene Column	Toluene Column	Xylene Column
Non-Aromatic	0.35	0.68	1.19
Benzene	56.10	0.83	0.03
Toluene	26.41	63.47	0.02
Ethylbenzene	9.41	19.90	56.10
p-Xylene	1.43	2.70	7.61
m-Xylene	3.56	7.31	20.59
o-Xylene	1.62	2.99	8.42
HNK(C9+)	1.12	2.12	6.04

the numbers of trays for each column are more or less than



(Figure 1) Schematic Flow Diagram of BTX Plant

The feeds to each column are composed of  $C_6 \sim C_{10}$  hydrocarbons. The composition of each feed is shown in Table 1. The components' volatility of the feeds is similar to one another and the range of boiling point is narrow. In the actual operation, the purity of products from each column should be maintained at more than 99.9%. For these reasons,

70.

BP method is based on the fact that the sum of each component's mol percent computed from thermodynamical relations is equal to one. Actually the range of boiling point of each component is very narrow and the temperature at each tray is much influenced by the composition of liquid

and vapor phases at the tray. SR method uses vapor flow rate as the tearing variable and is proper to the process which has wide range of boiling point. SC method was developed for modeling the three-phase distillation column and the reactive distillation column[1]. For the characteristics of the BTX plant is proper to BP method, we employed BP(Boiling Point) method to model and simulate the fractionation unit.

In modeling and simulation of BTX plant the main difficulties are how to apply proper stage efficiency and how to deal with HNK(heavy non-key) components.

Generally the column efficiency sets out from the fact that the distribution coefficient computed from the phase equilibrium gives higher composition values than actual values. A method based on Murphree efficiency generally has been used so far but in the method there is no consideration of each stage's position and the ratio of components' mol percent. Therefore we employed vaporization efficiency suggested by Seader[3].

In BTX plant the concentration of HNK is relatively low but the existence of HNK's affects to temperature and mass transfer rate in the whole column. Identification of HNK is very difficult. Considering the fact that HNK is mainly composed of C<sub>9</sub> and C<sub>10</sub>'s, we could compute average molecular weight and acentric factor of HNK's.

In the simulation we used C++ as main programming language. In the actual operation of the plant dynamic simulations are seldom used if ever and so we focused on steady-state simulations of the plant.

## 2. Mathematical Model for Distillation Columns

### (1) Theoretical Model for an Equilibrium Stage

We consider a general, continuous, steady-state vapor-liquid separator consisting of a number of stages. Figure 2 shows a typical stage of the distillation column. Assuming that phase equilibrium is achieved at each stage and that no chemical reactions occur, we can set up relevant material and energy balances and required thermodynamical relationships.

*component material balance :*

$$L_{j-1}x_{i,j-1} + V_{j+1}y_{i,j+1} + F_jz_{i,j} - (L_j + U_j)x_{i,j} - (V_j + W_j)y_{i,j} = 0 \tag{1}$$

*equilibrium relationship :*

$$y_{i,j} - K_{i,j}x_{i,j} = 0 \tag{2}$$

*summation equations :*

$$\begin{aligned} \sum_i y_{i,j} - 1.0 &= 0 \\ \sum_i x_{i,j} - 1.0 &= 0 \end{aligned} \tag{3}$$

*energy balance :*

$$L_{j-1}H_{L,j-1} + V_{j+1}H_{V,j+1} + F_jH_{F,j} - (L_j + U_j)H_{L,j} - (V_j + W_j)H_{V,j} - Q_j = 0 \tag{4}$$

### (2) Mathematical Formulation using Tridiagonal Matrix

The modern equation-tearing procedures developed recently are readily programmed, show rapid convergence and require a minimum computer storage. Modification of material balance equation (1) results in tridiagonal matrix form. By selecting T<sub>i,j</sub> and V<sub>i,j</sub> as the tear variables, we can tear the tridiagonal matrix form in which the material balance remains linear with respect to unknown liquid compositions[6]. Results of formulation can be arranged as equation (5).

$$A_j x_{i,j-1} + B_{i,j} x_{i,j} + C_{i,j} x_{i,j+1} = D_{i,j} \tag{5}$$

where

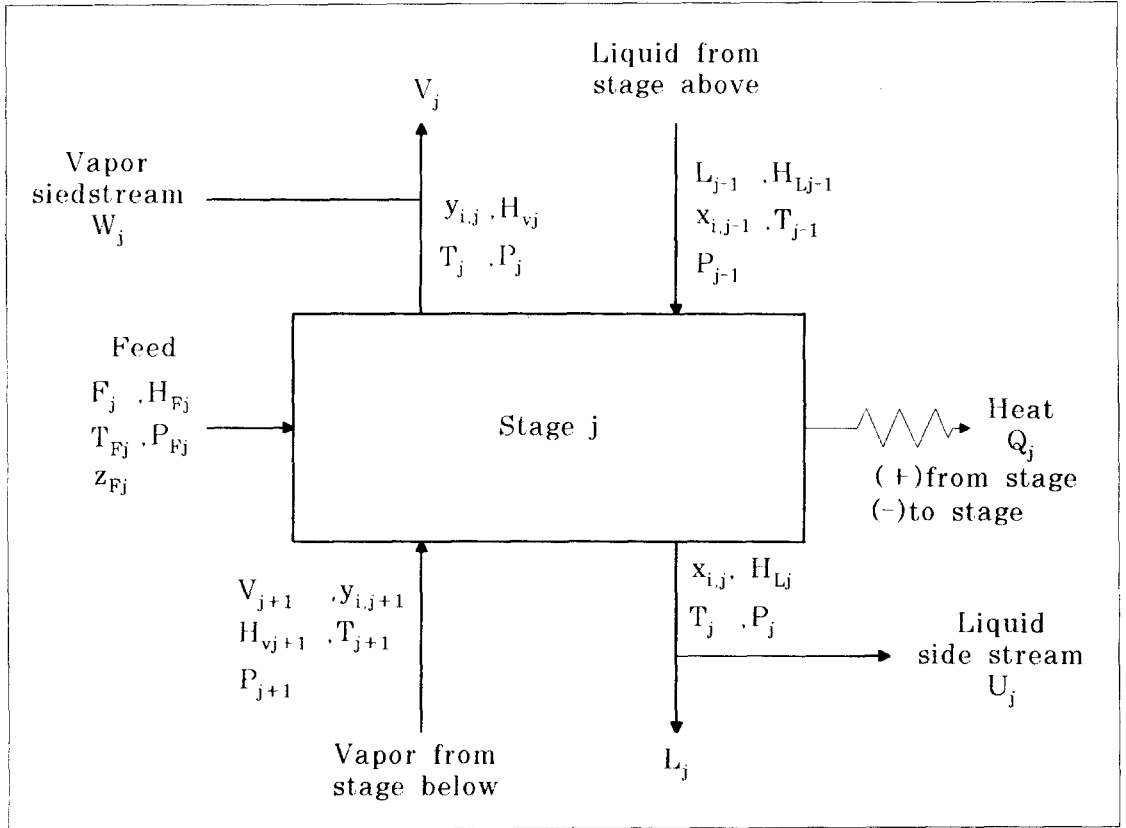
$$A_j = V_j - V_1 + \sum_{n=1}^{j-1} (F_n - U_n - W_n) ; 2 \leq j \leq N$$

$$B_{i,j} = - [ V_{j+1} - V_1 + U_j + (V_j + W_j) K_{i,j} + \sum_{n=1}^j (F_n - U_n - W_n) ] ; 1 \leq j \leq N$$

$$C_{i,j} = V_{j+1} K_{i,j+1} ; 1 \leq j \leq N-1$$

$$D_{i,j} = - F_j z_{i,j} ; 1 \leq j \leq N$$

Equation (5) can be rearranged in the matrix form.



(Figure 2) Schematic Diagram of an Equilibrium Stage

$$\begin{pmatrix} B_{i,1} & C_{i,1} & 0 & 0 & 0 & 0 \\ A_2 & B_{i,2} & C_{i,2} & 0 & 0 & 0 \\ 0 & A_3 & B_{i,3} & C_{i,3} & 0 & 0 \\ 0 & 0 & \vdots & \vdots & \vdots & 0 \\ 0 & 0 & 0 & A_{N-1} & B_{i,N-1} & C_{i,N-1} \\ 0 & 0 & 0 & 0 & A_N & B_{i,N} \end{pmatrix} \begin{pmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,3} \\ \vdots \\ x_{i,N-1} \\ x_{i,N} \end{pmatrix} = \begin{pmatrix} D_{i,1} \\ D_{i,2} \\ D_{i,3} \\ \vdots \\ D_{i,N-1} \\ D_{i,N} \end{pmatrix} \quad (6)$$

The above matrix equation can be rewritten by using Thomas algorithm.

$$\begin{pmatrix} 1 & P_{i,1} & 0 & 0 & 0 & 0 \\ 0 & 1 & P_{i,2} & 0 & 0 & 0 \\ 0 & 0 & 1 & P_{i,3} & 0 & 0 \\ 0 & 0 & 0 & \vdots & \vdots & 0 \\ 0 & 0 & 0 & 0 & 1 & P_{i,N-1} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,3} \\ \vdots \\ x_{i,N-1} \\ x_{i,N} \end{pmatrix} = \begin{pmatrix} q_{i,1} \\ q_{i,2} \\ q_{i,3} \\ \vdots \\ q_{i,N-1} \\ q_{i,N} \end{pmatrix} \quad (7)$$

where

$$P_{i,1} = C_{i,1} B_{i,1}^{-1}, P_{i,j} = C_{i,1} (B_{i,j} - P_{i,j-1} A_j)^{-1}$$

$$; j = 2, 3, \dots, N-1$$

$$q_{i,1} = D_{i,1} B_{i,1}^{-1}, q_{i,j} = (D_{i,j} - q_{i,j-1} A_j) (B_{i,j} - P_{i,j-1} A_j)^{-1}$$

$$; j = 2, 3, \dots, N$$

From the equation (7) we can easily obtain liquid composition as

$$\begin{aligned} x_{i,N} &= q_{i,N} \\ x_{i,j-1} &= q_{i,j-1} - P_{i,j-1} x_{i,j} \end{aligned} \quad (8)$$

The above formulation is highly efficient, requires a minimum of computer storage, and is superior to alternative

matrix-inversion routines. For these reasons we apply this algorithm in the modeling and simulation of BTX plant.

**(3) Calculation of Enthalpy and K values**

For the computation of enthalpy and K values we employed SRK(Soave-Redlich-Kwong) equation developed by Soave [6]. He added the Pitzer acentric factor to the RK equation because of the fact that RK equation can not predict vapor pressure accurately. By combining other thermodynamic equations with SRK equation, we can get the following nonlinear equations.

$$Z^3 - Z^2 + (A-B-B^2)Z - AB = 0 \tag{9}$$

$$K_i = (\hat{\varphi}_i)_L(\hat{\varphi}_i)_V^{-1} \tag{10}$$

subject to

$$\ln(\hat{\varphi}_i) = (Z-1)B_iB^{-1} - \ln(Z-B) - AB^{-1}(2\sqrt{A_iA^{-1}} - B_iB^{-1}) \ln(1+Z^{-1}) \tag{11}$$

$$H = H_V^0 + RT \left\{ Z-1-B^{-1} \ln(1+BZ^{-1}) \sum_{i=1}^C \sum_{j=1}^C y_i y_j A_{ij} (1-0.5m_i \sqrt{T_i a_i^{-1}} - 0.5m_j \sqrt{T_j a_j^{-1}}) \right\} \tag{12}$$

Before iterational computation we must set an initial K value. Antoine equation was used in the initialization. For the computation of enthalpy and K values, we used Newton-Raphson method which requires the differentiation of Z and K with respect to temperature. This method finds the solutions very fast but has a defect of occasional overflows.

**(4) HNK Handling and Determination of Efficiency**

HNK in BTX plant was found to be mainly composed of C<sub>9</sub> and C<sub>10</sub>. Therefore we can choose two components that represent characteristics of HNK's. In choosing those components, the following two methods can be used.

$$M.W_{avg} = \sum_i (M.W_i \times mol\%)$$

$$or \omega_{avg} = \sum_i (\omega_i \times mol\%) \tag{13}$$

The acentric factor,  $\omega'$ , has more significant effects to K values than molecular weight and so adequately characterizes the system for hydrocarbon mixtures the compositions of which are known.

In simulation, K values of each component are calculated at each stage and efficiency is multiplied to these K values.

$$K_i = \exp[\ln(\hat{\varphi}_i)_L(\hat{\varphi}_i)_V^{-1}] \times Efficiency_i \tag{14}$$

For the component which shows higher volatility than any other components the value of the efficiency computed is close to 1. Approximate efficiency is given by

$$Efficiency_i = M.W_i \sum_i (M.W_i x_{i,j}) \text{ or } \omega_i \sum_i (\omega_i x_{i,j}) \tag{15}$$

But this efficiency may be greater than 1, and we regarded the efficiency which has the highest value as 1 and recalculated other component efficiency relative to that value. Using this revised efficiency we could get good results.

**3. Proposed Algorithm**

The proposed BP algorithm can be summarized as following :

1. Specify  $N, F_j, z_{i,j}, U_j, W_j, Q_j, P_{Fj}, P_j, T_{Fj}$ , and  $V_1$ .
2. Specify type of condenser and compute  $L_N$  from overall mass balance ; if total condenser is used,  $V_1=0$ .

$$L_N = \sum_{i=1}^N (F_j - U_j - W_j) - V_1$$

3. Specify  $L_1$  or reflux ratio.
4. Compute  $V_2 = V_1 + L_1 + U_1 - F_1$ .
5. Provide initial guesses ( $k=0$ ) of tear variables  $T_j$  and  $V_j$ .
6. Set index  $k=1$  to indicate the first column iteration.
7. Compute  $K_{i,j}$  using SRK equation ; if  $k=1$ , use Antoine equation.
8. compute  $x_{i,j}$  by equation (8).

9. To force  $\sum_i x_{ij} = 1$  at each stage  $j$ , normalize values by the replacement.

$$x_{ij} = x_{ij}(\sum_i x_{ij})^{-1}$$

10. Compute a new set of values of  $T_j^{(k)}$  tear variables by using  $K_{ij}$  computed by SRK equation and the relationship,  $\sum K_{ij} x_{ij} = 1.0$ .
11. Compute  $y_{ij}$  by equation (2).
12. Compute a new set of variables of the  $V_j$  tear variables by energy balance.
13. Check to determine if the new sets of tear variables  $T_j^{(k)}$  and  $V_j^{(k)}$  are within some prescribed tolerance of sets  $T_j^{(k-1)}$  and  $V_j^{(k-1)}$  used to initiate the current column iteration. A possible convergence criterion is

$$\sum_{j=1}^N \left\{ (T_j^{(k)} - T_j^{(k-1)}) / T_j^{(k)} \right\}^2 + \sum_{j=3}^N \left\{ (V_j^{(k)} - V_j^{(k-1)}) / V_j^{(k)} \right\}^2 \leq 10^{-2} \times N$$

or

$$\sum_{j=1}^N \left\{ T_j^{(k)} - T_j^{(k-1)} \right\}^2 \leq 10^{-2} \times N$$

14. If the convergence criterion is met, compute values of  $L_j$  from component mass balance at each stage and  $Q_1$  and  $Q_2$  from equation (4). Otherwise, set  $k = k + 1$  and repeat steps 7 to 14.

## 4. Results and Discussions

The specifications and normal operating conditions of the fractionation columns are shown in Table 2. Total capacity of BTX plant is determined by benzene column feed. 100% feed load of benzene column is equivalent to 25,000kg/hr. Normal operating range is 50~80% feed and the simulation is carried out with 63.5% load. Feed flow rate and reflux ratio are main control variables of BTX plant. The feed flow rate to each column is determined by prior unit and so reflux ratio is an actual control variable. Desired product purity can be achieved by proper reflux ratio which is determined by using the temperature of each column. Because the bottom

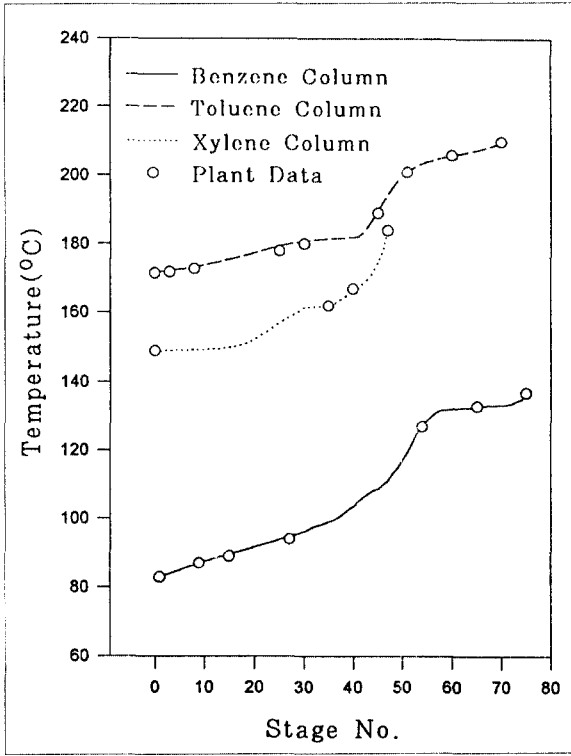
(Table 2) BTX Plant Specification

Variable \ Column	Benzene Column	Toluene Column	Xylene Column
Feed Flow Rate (kg/hr)	15,600	6,600	2,600
Feed Temperature (°C)	160	136	208
Feed Pressure (atm)	13.46	6.97	3.78
Top Pressure (atm)	1.02	4.40	1.35
Bottom Pressure (atm)	1.42	4.85	1.65

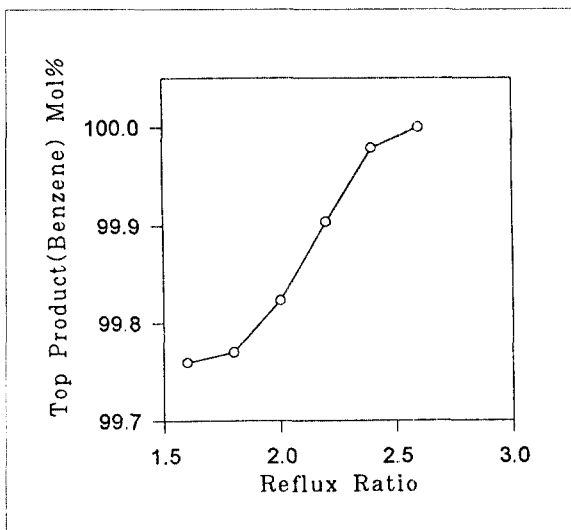
section of each column has much more heavy components and operates in higher pressure than the upper section, the temperature of each column increases with respect to stage number. The toluene column operates at relatively higher pressure than other columns and so the temperature of toluene column is higher than that of others. The temperature profiles of benzene, toluene and xylene columns are shown in Fig. 3, as can be seen, the simulation results show good agreement with actual plant operation data.

In operating the distillation column, the most important control variable is reflux ratio. By changing reflux ratio, we can get the desired product purity and reduce operating cost. In benzene and toluene columns, the normal range of reflux ratio is about 2.0. But in xylene column, the reflux ratio ranges from 0.8 to 1.6. The purity of top product of benzene and toluene columns should be maintained at 99.9%. But the top product purity of xylene column is not so important because the top product is mainly composed of four components. Fig. 4 to Fig. 6 show concentrations of top products (mol%) with respect to reflux ratio changes in each column. It was found that the reflux ratio in benzene and toluene columns should be maintained at 2.2 and the normal operating condition of reflux ratio can often cause off-specification of purity.

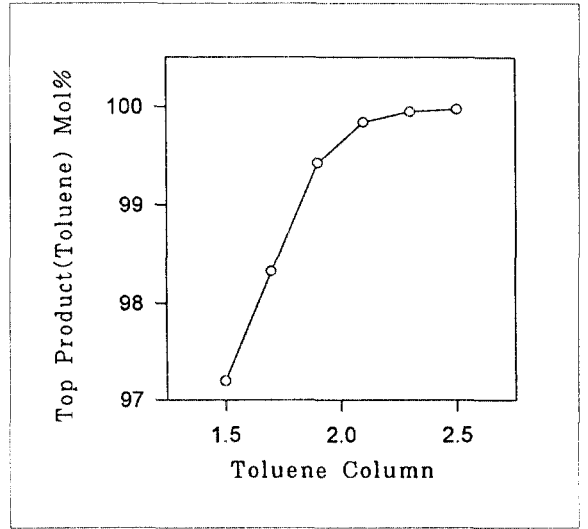
Fig. 7 to Fig. 9 show vapor and liquid flow rates in each column. From Fig. 7 we can see that the feed of benzene



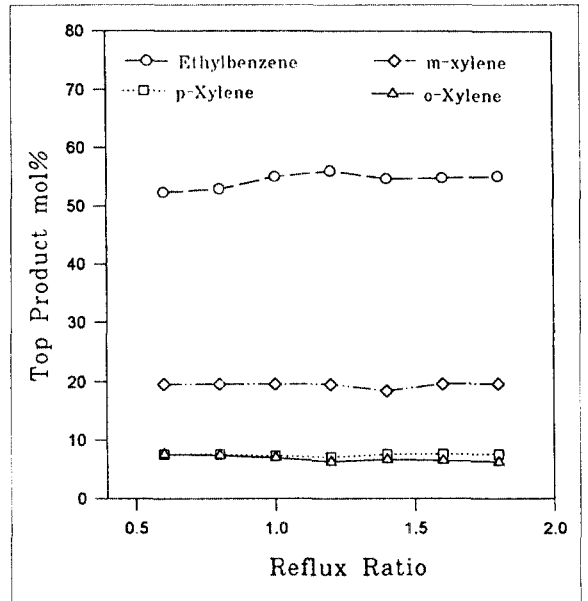
<Figure 3> Temperature Profile of BTX Plant



<Figure 4> Top Product (Benzene) Mo1% vs. Reflux Ratio in Benzene Column

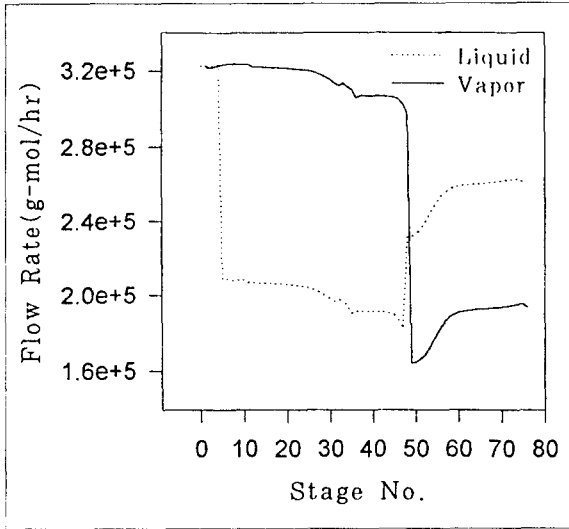


<Figure 5> Top Product (Toluene) Mo1% vs. Reflux Ratio in Benzene Column

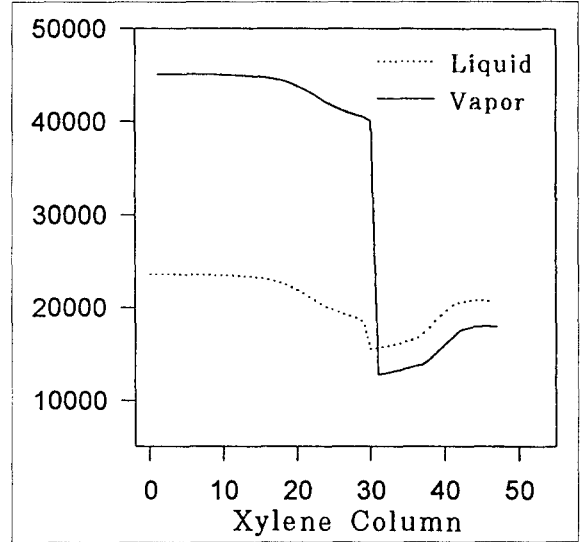


<Figure 6> Top Product Mo1% vs. Reflux Ratio in Xylene Column

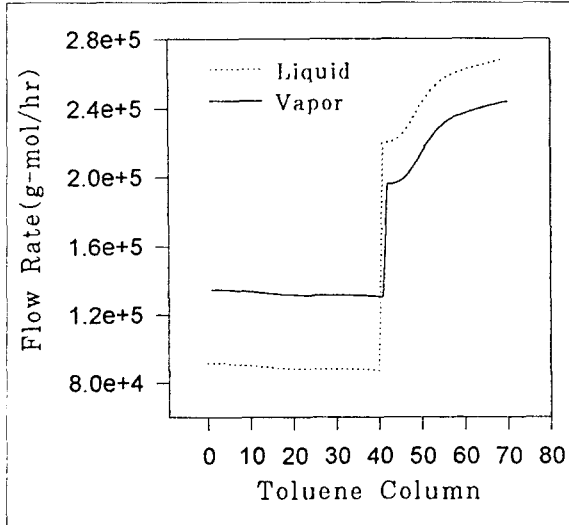
column separates into two phases and that vapor and liquid flow rates near the feed stage increase. In toluene column



〈Figure 7〉 Vapor & Liquid Flow Rate(g-mol/hr) vs. Stage No. in Benzene Column



〈Figure 9〉 Vapor & Liquid Flow Rate(g-mol/hr) Reflux Ratio in Xylene Column



〈Figure 8〉 Vapor & Liquid Flow Rate(g-mol/hr) vs. Stage No. in Toluene Column

(Fig. 8), the feed remains as liquid phase so the vapor and liquid flow rates just below the feed stage increase. In this case, the feed is not vaporized at the feed stage because of the fact that the temperature of the feed stage is about 180°C

which is a little bit higher than the flash temperature of the feed. From Fig. 9 we can see that xylene column shows opposite behavior to toluene column. Also we can get the design specification of distillation through vapor and liquid flowrates.

In the operation of distillation columns, the energy is mainly consumed by cooling water and steam and can be mainly controlled by reflux ratio. Cooling water is used to condense top vapor and steam is used to vaporize bottom liquid. The necessary condenser and reboiler heat duties is calculated from multiplication of flow rate and latent heat at top and bottom stages and increases as feed increases as can be seen in Table 3. Energy duties can decrease by lower reflux ratio but this can cause off-specification of purity. Based on the simulation results optimization study of the whole BTX plant is planned in the future

## 5. Conclusions

Modeling and simulation was performed for the actual BTX fractionation plant. Because the fractionation unit of benzene-toluene-xylene plant has a narrow range of boiling point and doesn't



(Table 3) Reboiler & Condenser Heat Duty(Kcal\*10<sup>4</sup>/hr) vs. Feed Load

		52%	61%	73%	85%	100%
Benzene	Reboiler	30.24	37.8	45.36	52.92	63
	Column	60.8	80.6	95.8	110.9	133.6
Toluene	Reboiler	34	39.56	45.36	50.4	64.26
	Column	20.16	24.44	27.72	30.24	39.06
Xylene	Reboiler	4.79	6.05	6.80	7.81	10.84
	Column	7.06	9.83	10.58	12.35	17.14

doesn't have any sidecut and side reboiler, we employed boiling point estimation method in the modeling and simulation of the plant. Soave-Redlich-Kwong equation was used in the computation of thermodynamical properties. We solved resulting nonlinear equations by using Newton-Raphson method which is known to show fast convergence. Results of simulations showed good agreement with actual plant operation data.

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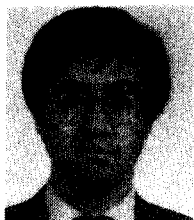
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