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OPTIMIZATION OF FRACTIONATION OPERATION IN THE BENZENE-TOLUENE-XYLENE PLANT

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Abstract – A steady-state optimization for the fractionation unit of an industrial benzene-toluene-xylene (BTX) plant was developed. Because the fractionation unit of the BTX plant has narrow ranges of boiling point and doesn't have any sidecut and side reboiler, we employed the boiling point estimation method in the modeling and simulation of the unit. The well-known Soave-Redlich-Kwong state equation was employed to compute required thermodynamic properties. The results of simulations showed very good agreement with the actual operation data. The objective of the optimization was to maximize profit of fractionation unit. The successive quadratic programming algorithm was utilized and objective functions for each fractionation column were set up based on utility and operation costs and selling prices of products. The graphical user interface of the optimization system was developed to provide convenience and flexibility in actual applications.

Key words: *Fractionation Unit, Simulation, BP Method, Optimization, SQP, Reflux Ratio*

INTRODUCTION

In the operation of chemical plants, optimal operating conditions should be maintained to maximize profits as well as to minimize costs. An optimization system for a chemical plant is usually based on the model of the plant. Therefore the development of the optimization system for a chemical plant consists of identification of the plant model and application of suitable optimization algorithms. The main purpose of the present work is to develop an optimization system to achieve optimal operation for the fractionation unit of an industrial benzene-toluene-xylene (BTX) plant.

The BTX plant considered in the present work consists of hydrotreating unit, extraction unit, fractionation unit and hydrodealkylation unit. Among these four units, the fractionation unit is by far the most important unit and economics of the BTX plant depend heavily on it. In this work the fractionation unit which consists of three distillation columns is considered. The model of the fractionation unit was developed based on actual operation data.

So far various methods have been developed for modeling of distillation processes. Summary of typical calculation methods are shown in Table 1.

Some of these methods are commercially available but usefulness of those methods depends on the characteristics of the processes employed. Relaxation is applicable to solve the nonideal and reactive systems. 2N Newton is suitable for the nearly ideal cases and processes with many trays. Algorithms of the global Newton is not suitable to solve distillation problems with a great number of components on small computers because of the requirements of large computer memory. Inside-out method allows a wide variety of performance specifications and provides good speed, but it is rather complicated.

Modeling of the fractionation unit of the BTX plant requires accurate thermodynamic properties of each chemical compounds and knowledge of operational constraints. In this present work modifications of the existing modeling method were performed by employing suitable thermodynamic relationships and various operational constraints.

Fig. 1 shows the flow diagram of the fractionation unit considered in the present work. The fractionation unit consists of three distillation columns, each of which has 75, 70, and 47 trays respectively. Benzene, toluene and xylene are obtained as top products of each column. The feeds to each column are composed of C_6-C_{10} hydrocarbons. Table 2 shows the com-

Table 1. Typical methods of distillation calculation

Method	References
Boiling point	[Holland, 1981]
Relaxation	[Ketchum, 1979]
2N Newton	[Tomich, 1970; Holland, 1981]
Global Newton	[Naphtali et al., 1971; Holland, 1981; Goldstein et al., 1970]
Inside-out	[Boston, 1980; Russell, 1983]

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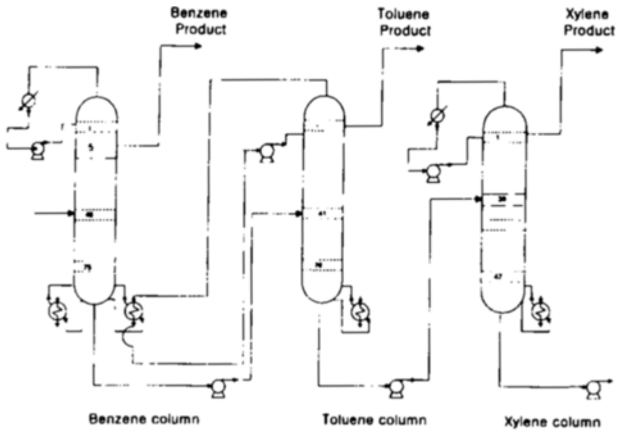

Fig. 1. Schematic flow diagram of the fractionation unit.

Table 2. Feed compositions (mole %) of fractionation columns

Component	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(C_{9+})	1.12	2.12	6.04

positions of each feed. The relative volatilities of the feeds are similar to one another and the range of boiling points is narrow. In the operation, the purity of products from each fractionation column should be maintained at more than 99.9 %.

The narrow range of boiling points of the feeds enables us adoption of well-known BP (Boiling Point) method to model and to simulate the fractionation unit. The temperature at each tray is much influenced by the composition of liquid and vapor phases at the tray.

In modeling and simulation of the fractionation unit the main issues to be investigated are how to apply proper stage efficiency and how to deal with HNK (heavy non-key). Generally the column efficiency sets out from the fact that the distribution coefficients computed from the phase equilibrium relationships give higher composition values than actual values. A method based on Murphree efficiency has been generally used so far but the method does not take account of the position of each stage's position and of the composition ratio of each component. In this work we employed vaporization efficiency suggested by Holland et al. [1983].

In the fractionation unit the concentration of HNK is relatively low but the existence of HNK's affects to temperature and mass transfer in the whole columns. Considering the fact that HNK is mainly composed of C_9 and C_{10}'s, we computed average molecular weight and acentric factor of HNK's based on appropriate typical C_9 and C_{10} materials.

In the optimization the construction of objective functions is very important. We used reflux ratios and product outputs as control variables which affect on energy costs and the purity of products. In the computation we employed SQP (Successive Quadratic Programming) algorithm to identify optimal operating conditions of the fractionation unit. In the SQP algorithm the object function is approximated as a quadratic function and the constraints as linear functions so that the quadratic programming method could be used recursively.

C was used as the main computer language to construct program blocks and to develop graphical user interfaces. In the design of the graphical user interfaces the needs and recommendations of the plant operators and engineers were fully incorporated.

MODELING OF FRACTIONATION COLUMNS

1. Mathematical Formulations

We consider a general, continuous, steady-state column consisting of a number of stages. Fig. 2 represents typical stage of a fractionation column. The Modeling of a distillation column based on the steady-state material and energy balances is well-known technique and we can find summary of various modeling methods from many literatures [Henley and Seader, 1981; Kister, 1992].

Assuming that phase equilibrium is achieved at each stage and that no chemical reactions occur, we can set up the relevant material and energy balances and required thermodynamic relationships.

Component material balance:

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

Equilibrium relationship:

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

Summation equations:

$$\sum_i y_{i,j}-1.0=0$$

$$\sum_i x_{i,j}-1.0=0 \tag{3}$$

Energy balance:

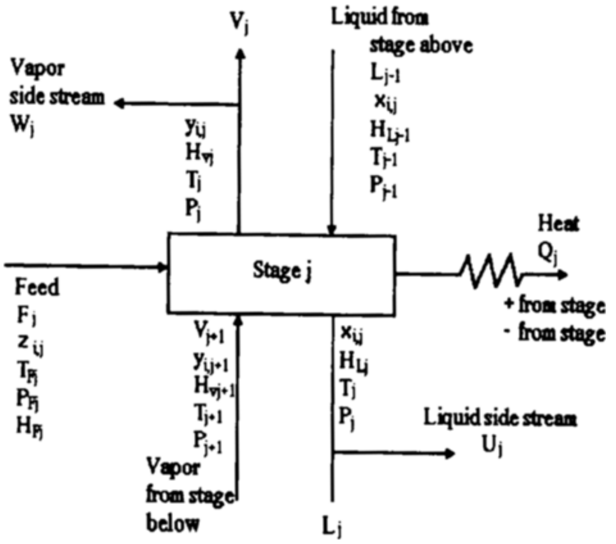

Fig. 2. Schematic diagram of an equilibrium stage.

$$L_{j-1}\,H_{Lj-1}+V_{j+1}\,H_{Vj+1}+F_j\,H_{Fj}-(L_j+U_j)H_{Lj}-(V_j+W_j)H_{Vj}-Q_j=0 \tag{4}$$

where L_j, V_j, F_j, U_j and W_j represent internal liquid flow rate, vapor flow rate, feed flow rate, liquid sidecut and vapor sidecut at stage j respectively, H_{Fj}, H_{Lj} and H_{Vj} are molar enthalpy of feed, liquid and vapor phase and Q_j is heat duty. For component i and stage j $x_{i,j}$, $y_{i,j}$ and $z_{i,j}$ stand for liquid, vapor and feed composition and $K_{i,j}$ is equilibrium constant. The Modification of material balance Eq. (1) results in tridiagonal matrix form. By selecting temperature (T_j) and vapor flow rate (V_j) as tear variables, we can tear the tridiagonal matrix form in which the material balance remains linear with respect to unknown liquid compositions. Results of formulation can be rearranged by using Thomas algorithm as

$$\begin{bmatrix} 1 & P_{i,1} & 0 & 0 & 0 & 0 \\ 0 & 1 & P_{i,2} & 0 & 0 & 0 \\ 0 & 0 & 1 & P_{i,3} & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & 1 & P_{i,N-1} \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_{i,1} \\ x_{i,2} \\ x_{i,3} \\ \vdots \\ x_{i,N-1} \\ x_{i,N} \end{bmatrix} = \begin{bmatrix} q_{i,1} \\ q_{i,2} \\ q_{i,3} \\ \vdots \\ q_{i,N-1} \\ q_{i,N} \end{bmatrix} \tag{5}$$

where

$$P_{i,1}=\frac{C_{i,1}}{B_{i,1}},\ P_{i,j}=\frac{C_{i,1}}{B_{i,j}-P_{i,j-1}A_j} \quad (j=2,3,\cdots,N-1)$$

$$q_{i,1}=\frac{D_{i,1}}{B_{i,1}},\ q_{i,j}=\frac{D_{i,j}-q_{i,j-1}A_j}{B_{i,j}-P_{i,j-1}A_j} \quad (j=2,\ 3,\ \cdots,\ N)$$

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

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

$$C_{i,j}=V_{j+1}K_{i,j+1} \quad (1\le j\le N-1)$$

$$D_{i,j}=-F_j\,z_{i,j} \quad (1\le j\le N).$$

From the Eq. (5) we can readily obtain liquid compositions as

$$x_{i,N}=q_{i,N}$$
$$x_{i,j-1}=q_{i,j-1}-P_{i,j-1}\,x_{i,j}. \tag{6}$$

The above formulation is highly efficient, requires minimum computer storage, and is superior to alternative matrix-inversion routines.

2. Thermodynamic Properties

For the computation of enthalpy and K values we employed RK (Redlich-Kwong) state equation modified by Soave[1972]. From the SRK equation; we can easily get a third-order nonlinear algebraic equation which can be solved by using appropriate numerical method such as Newton-Raphson algorithm. In the application of the Newton-Raphson method evaluation of distribution coefficients K_is and differentiation of them are required. All the related properties and relationships can be summarized as following using compressibility factor (Z), and fugacity coefficient ($\hat{\psi}$).

Distribution coefficient:

$$K_i=\frac{(\hat{\phi}_i)_L}{(\hat{\phi}_i)_V} \tag{7}$$

Enthalpy:

$$H=H_V^o+RT\left[Z-1-\frac{1}{B}\ln\left(1+\frac{B}{Z}\right)\sum_{i=1}^{C}\sum_{j=1}^{C}y_iy_jA_{ij}\right.$$
$$\left.\left(1-\frac{m_i}{2}\sqrt{\frac{T_{ri}}{a_i}}\ 1-\frac{m_j}{2}\sqrt{\frac{T_{rj}}{a_j}}\right)\right] \tag{8}$$

Differentiation of K_i:

$$\frac{dK_i}{dT}=K_i\left\{\frac{d}{dT}\ln(\hat{\phi}_i)_L-\frac{d}{dT}\ln(\hat{\phi}_i)_V\right\} \tag{9}$$

where

$$\ln(\hat{\phi}_i)=(Z-1)\,\frac{B_i}{B}-\ln(Z-B)-\frac{A}{B}\left(2\sqrt{\frac{A_i}{A}}-\frac{B_i}{B}\right)$$
$$\ln\left(1+\frac{B}{Z}\right) \tag{10}$$

$$\frac{d}{dT}\ln(\hat{\phi}_i)=\left[\frac{B_i}{B}-\frac{1}{(Z-B)}+\frac{B}{Z(Z+B)}\left(2\sqrt{AA_i}-\frac{AB_i}{B}\right)\right]$$
$$\times\frac{(2A-B-2B^2)Z-3AB}{T(3Z^2-2Z+A-B-B^2)}-\frac{1}{T}\frac{B_i}{B}\left[(Z-1)+\frac{A}{B}\ln\left(1+\frac{B}{Z}\right)\right]$$
$$-\frac{1}{T}\left[\frac{(1-Z)B_i}{B}+\frac{B}{(Z-B)}+\left(\frac{2\sqrt{AA_i}}{B}-\frac{2AB_i}{B^2}\right)\ln\left(1+\frac{B}{Z}\right)\right.$$
$$\left.-\frac{1}{(Z+B)}\left(2\sqrt{AA_i}-\frac{AB_i}{B}\right)\right]+\frac{4}{T}\frac{\sqrt{A_iA}}{B}\ln\left(1+\frac{B}{Z}\right)$$
$$-\frac{2AB_i}{TB^2}\ln\left(1+\frac{B}{Z}\right)$$

$$A=\sum_{i=1}^{c}\sum_{j=1}^{c}y_iy_jA_{ij}\ \text{or}\ \sum_{i=1}^{c}\sum_{j=1}^{c}x_ix_jA_{ij}\ \text{and}\ A_{ij}=\sqrt{A_iA_j}$$

$$a_i=(1+m_i(1-\sqrt{T_{r_i}}))^2\ \text{for component i}$$

$$A_i=0.42747\,a_i\,\frac{P_{r_i}}{T_{r_i}}\ \text{for component i}$$

$$B=\sum_{i=1}^{c}y_i\,B_i\ \text{or}\ \sum_{i=1}^{c}x_i\,B_i$$

$$B_i=0.08664\,\frac{P_{r_i}}{T_{r_i}}$$

$$H_{iV}^o=\int_{T_*}^{T}C_{P_*}^o\ dT$$

The antoine equation was used in the initialization of distribution coefficients.

The HNK in the fractionation unit was found to be mainly composed of C_9's and C_{10}'s. Therefore we chose two typical C_9 and C_{10} components which represented characteristics of HNK very well. The choice of the components was based on the following criterion.

$$\omega_{avg} = \sum_i (\omega_i \times \text{mol\%}) \tag{11}$$

The acentric factor, ω, has more significant effects on K values than the molecular weight and adequately represents the compositions of hydrocarbon mixtures. K_i values of each component are calculated at each stage and multiplied by stage efficiency E_i.

$$K_i = \exp\left[\ln \frac{(\hat{\phi}_i)_L}{(\hat{\phi}_i)_V}\right] \times E_i \tag{12}$$

For the component which has higher volatility than any other components the value of the efficiency computed was close to 1. The approximate component efficiency can be obtained by using molecular weight or acentric factor of each component. During the computation when a component efficiency is greater than 1, we regarded the efficiency which has the highest value as 1 and recalculated the efficiencis of the other components.

3. Computational Procedure

(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; $V_1=0$ for total condenser.

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

(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 $K_{i,j}$; if k=1, use Antoine equation.

(8) compute $x_{i,j}$ by (6).

(9) To force $\sum_i x_{i,j} = 1$ at each stage j, normalize values by $x_{i,j} = \frac{x_{i,j}}{\sum_i x_{i,j}}$.

(10) Compute a new set of values of $T_j^{(k)}$ tear variables by using $K_{i,j}$ and the relationship $\sum_i K_{i,j}\, x_{i,j}=1.0$.

(11) Compute $y_{i,j}$ from (2).

(12) Compute a new set of variables of the V_j tear variables by energy balance.

(13) Check whether 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

$$\sum_{j=1}^{N}\left[\frac{T_j^{(k)} - T_j^{(k-1)}}{T_j^{(k)}}\right]^2 + \sum_{j=3}^{N}\left[\frac{V_j^{(k)} - V_j^{(k-1)}}{V_j^{(k)}}\right]^2 \le \varepsilon_1 \times N$$

$$\text{or } \sum_{j=1}^{N}\left[T_j^{(k)} - T_j^{(k-1)}\right]^2 \le \varepsilon_2 \times N$$

where ε_1 and ε_2 are very small number.

(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 Eq. (4). Otherwise set k=k+1 and return to step 7.

OPTIMIZATION OF FRACTIONATION OPERATION

1. SQP Method

In the fractionation operation the well-known SQP (Successive Quadratic Programming) method can be effectively used for the optimization. A typical SQP method can be formulated as following:

$$\text{Minimize: } s^T\nabla f(x) + \frac{1}{2}\, s^T\mathbf{B}s \tag{13}$$

$$\text{Subject to: } g_j(x)+s^T g_j(x) \ge 0 \qquad j=m+1, \ldots, p \tag{14}$$

$$h_j(x)+s^T\nabla h_j(x)=0 \qquad j=q, \ldots, m$$

where s the search direction, **B** a positive definite approximation of the Hessian, $g_j(x)$ inequality constraint and $h_j(x)$ is equality constraint.

The computational procedure for SQP method can be summarized as:

(1) Initialization (k=0): Choose r^0, x^0, B^0 (usually $\mathbf{B}^0=\mathbf{I}$).

(2) Calculate members of active set of constraints
Calculate the set of constraints, $\hat{h}(\mathbf{x}^k)$, if k=0, go to step 6.

(3) Termination

$$\frac{\|\mathbf{x}^k - \mathbf{x}^{k-1}\|}{\|\mathbf{x}^k\| + 1} < \varepsilon_1 \text{ for some prespecified tolerance } \varepsilon_1 > 0$$

$$|\hat{h}(\mathbf{x}^k)| < \varepsilon_j \text{ for some prespecified tolerance } \varepsilon_j > 0$$

where ε_1, ε_j are very small numbers.
Stop if both criteria are satisfied; otherwise continue.

(4) Update the approximate Hessian matrix;
use BFGS's method to update the approximate Hessian matrix.

$$\Delta\hat{\mathbf{H}}^k = \frac{\Delta\mathbf{g}^k(\Delta\mathbf{g}^k)^T}{(\Delta\mathbf{g}^k)^T\Delta\mathbf{x}^k} - \frac{\hat{\mathbf{H}}\Delta\mathbf{x}^k(\Delta\mathbf{x}^k)^T\hat{\mathbf{H}}^k}{(\Delta\mathbf{x}^k)^T\hat{\mathbf{H}}^k\Delta\mathbf{x}^k}$$

$$\Delta(\hat{\mathbf{H}}^k)^{-1} = \frac{[\Delta\mathbf{x}^k - (\hat{\mathbf{H}}^k)^{-1}\Delta\mathbf{g}^k](\Delta\mathbf{x}^k)^T + \Delta\mathbf{x}^k[\Delta\mathbf{x}^k - (\hat{\mathbf{H}}^k)^{-1}\Delta\mathbf{g}^k]^T}{(\Delta\mathbf{g}^k)^T\Delta\mathbf{x}^k}$$

$$- \frac{[\Delta\mathbf{x}^k - (\hat{\mathbf{H}}^k)^{-1}\Delta\mathbf{g}^k]^t\Delta\mathbf{g}^k\Delta\mathbf{x}^k(\Delta\mathbf{x}^k)^T}{[(\Delta\mathbf{g}^k)^T\Delta\mathbf{x}^k][(\Delta\mathbf{g}^k)^T\Delta\mathbf{x}^k]}$$

where bold $\Delta\mathbf{g}^k=\nabla_x L(\mathbf{x}^{k+1}, \mathbf{u}^{k+1}) - \nabla_x L(\mathbf{x}^k, \mathbf{u}^{k+1})$ with $s^k\,\Delta\mathbf{g} > 0$.

(5) Calculate **A**, **g**(x), and ∇f(**x**)

(6) Estimate the Lagrange multipliers to estimate the vector of Lagrange multipliers $\mathbf{u}^k$:

$$\left(\frac{r}{2}\mathbf{I} + \mathbf{A}\mathbf{B}^{-1}\mathbf{A}^T\right)\mathbf{u} = \mathbf{A}\mathbf{B}^{-1}\nabla\mathbf{f}(\mathbf{x}) - \hat{\mathbf{h}}(\mathbf{x})$$

(7) Calculate a new search direction $\mathbf{s}^k$ at $\mathbf{x}^k$ by

$$\mathbf{s}=\mathbf{B}^{-1}[\mathbf{A}^T\mathbf{u} - \nabla\, f(\mathbf{x})].$$

If a satisfactory search direction is not found, calculate a new r^k that satisfies following inequality equation and return to step 5.

$$-\frac{r}{2}\hat{\mathbf{h}}^T(\mathbf{x})\mathbf{u}-\hat{\mathbf{h}}^T(\mathbf{x})\hat{\mathbf{h}}(\mathbf{x})\leq 0$$

(8) Move a step in the $\mathbf{s}^k$ direction and calculate the step length λ^k along $\mathbf{s}^k$ by minimizing $P(\mathbf{x}^k+\lambda\mathbf{s}^k, r^k, \mathbf{u}^k)$.

(9) Let $\mathbf{x}^{k+1}=\mathbf{x}^k+\lambda^k\mathbf{s}^k$, k=k+1 and go to step 2.

2. Objective Function

In the fractionation unit the Objective Function (OF) is composed of profit and cost as

$$OF=(Profit-Cost)*(-1.0).$$

The cost consists of reboiling and condensing cost. These costs are mainly influenced by reflux ratio (L/D) and product output (D). The condensing cost C_C is given by

$$C_C=(D*L/D+D)*S_H \tag{15}$$

and the reboiling cost C_H is given by

$$C_H=V_S*S_H. \tag{16}$$

where V_S is steam flow rate going into reboiler, S_H is heating cost respectively. Besides profit and cost the compositions of each fractionation column were incorporated to the objective function to prevent the purity of overhead product from going down below standard value. Resulting objective functions for each column can be represented as following by using composition of overhead product (x_D) and feed cost (S_F).

Benzene Column:

$$OF=[17.9D-0.25(D*L/D+D)-1.88V_S+0.1\,x_D^2-3.7F*S_F]*(-1.0). \tag{17}$$

Toluene Column:

$$OF=[14.11D-0.89(D*L/D+D)-1.5V_S+0.1\,x_D^2-3.6F*S_F]*(-1.0). \tag{18}$$

Xylene Column:

$$OF=[27.09D-1.12(D*L/D+D)-1.83V_S+0.1\,x_D^2-3.9F*SF]*(-1.0). \tag{19}$$

As constraints for the optimization problem we consider the amount and purity of the overhead product and the feasible range of the reflux ratio. In the present work constraints can be summarized as:

$$F*x_D*0.99\leq D\leq F*x_D$$
$$R_{min}\leq L/D\leq R_{max}$$
$$0.999\leq x_D\leq 1.000 \text{ (Benzene and Toluene column)}$$
$$0.900\leq x_D\leq 1.000 \text{ (Xylene column)}$$

RESULTS AND DISCUSSIONS

In order to verify the models developed in the present study results of simulations were compared to actual operation data. Operating conditions of the fractionation unit are given in Table 3. The capacity of the fractionation unit depends on the feed

Table 3. Operating conditions of the fractionation unit

Variable	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

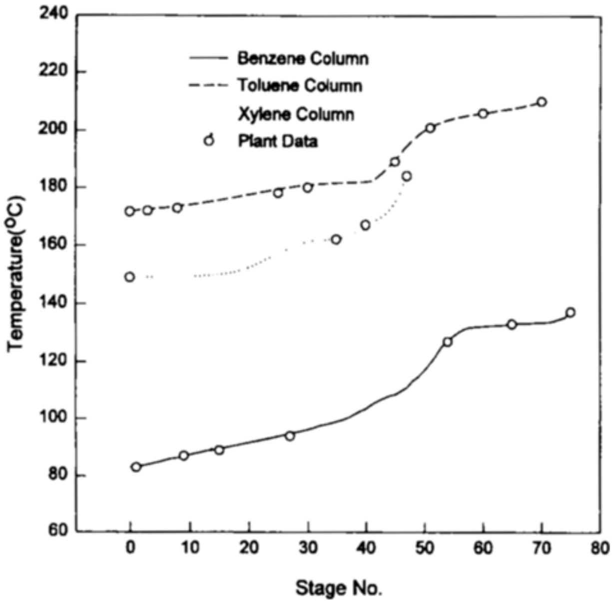

Fig. 3. Temperature profile of the fraction unit.

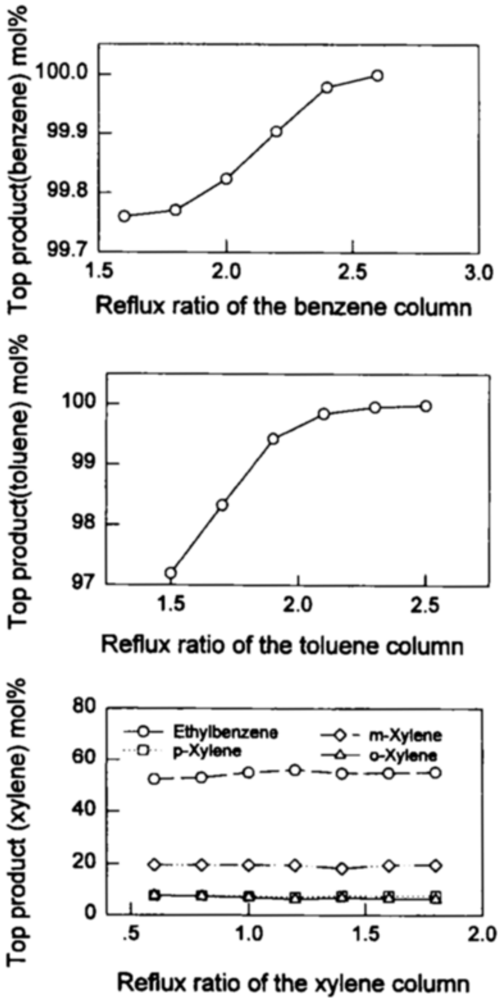

Fig. 4. Top product mol% vs. reflux ratio.

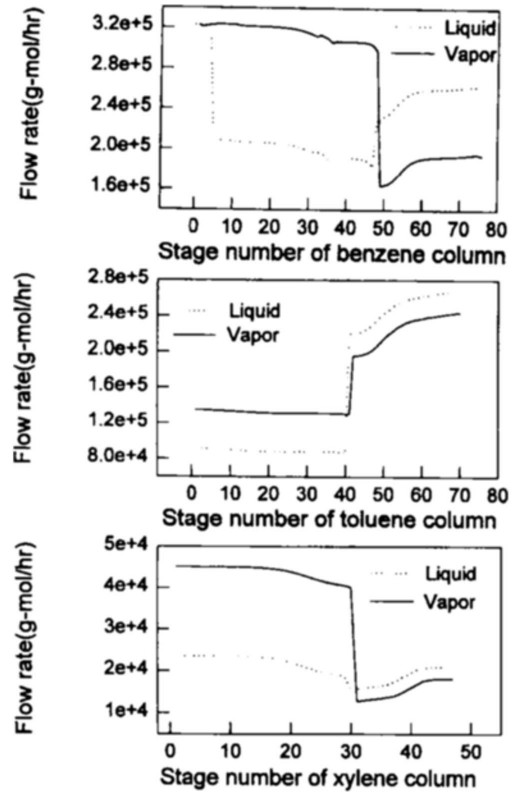

Fig. 5. Vapor & liquid flow rate vs. stage.

to the benzene column. 100 % feed load to the benzene column corresponds to 25,000 kg/hr. Normal operating range of the fractionation unit is 50-80% and simulations are based on 63.5 % load condition. The feed flow rate and reflux ratio are main control variables of the fractionation unit. In the usual operation the feed flow rate is determined by the prior plant, so the reflux ratio is the key control variable. The product purity should be maintained within the constraint which can be accomplished by proper reflux ratio.

The reflux ratio is determined based on the temperature profile of each column as shown in Fig. 3. As can be seen from Fig. 3, there is little discrepancy between the actual operation data and the results of simulations plotted by solid and dotted lines. This fact demonstrates the effectiveness of the fractionation model developed in the present study.

The normal operating range of reflux ratio of benzene and toluene columns is around 2.0 while that of the xylene column is from 0.8 to 1.6. The top product purity of benzene

Table 4. Reboiler & condenser heat duty (kcal*10^4/hr) vs. feed-load

Feed load	Benzene column		Toluene column		Xylene column	
(Kg/hr)	Reboiler	Condenser	Reboiler	Condenser	Reboiler	Condenser
13,160	30.24	60.8	34.0	20.16	4.79	7.06
15,430	37.8	80.6	39.56	24.44	6.05	9.83
18,470	45.36	95.8	45.36	27.72	7.03	10.31
21,500	52.92	110.9	50.4	30.24	8.91	13.59
25,300	63.0	133.6	64.26	39.06	10.84	17.14

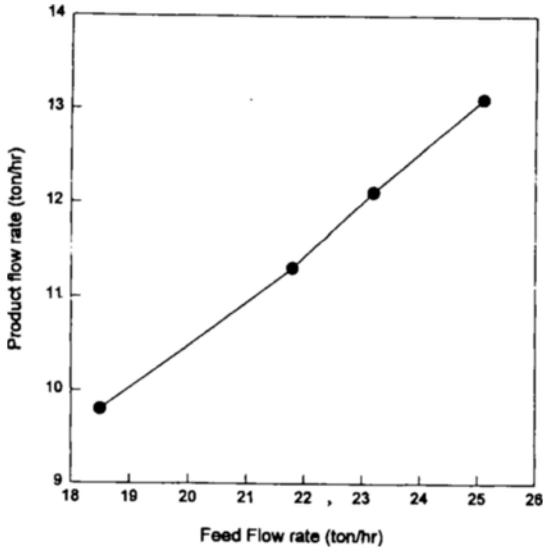

Fig. 6. Optimal production vs. feed change in benzene column.

and toluene columns should be maintained at least 99.9 %, but the top product purity of xylene column is not important because the product is mainly composed of four components.

Fig. 4 shows the relation between mole % of top product and changes of reflux ratio in each column. We have found that the reflux ratio should be maintained at least over 2.2 which is a little higher than the present operating range.

Fig. 5 shows vapor and liquid flow rates in each column. The sharp change of vapor and liquid flow rates of the benzene column near the feed stage is due to the fact that the feed to the benzene column separates into two phases. In toluene column, the feed remains as liquid phase and the vapor and liquid flow rates below the feed stage increase. The temperature of the feed stage is about 180 °C which is relatively higher than that of the feed and the flash doesn't occurs. The xylene column shows opposite characteristics to the toluene column because the temperature of the feed stage in

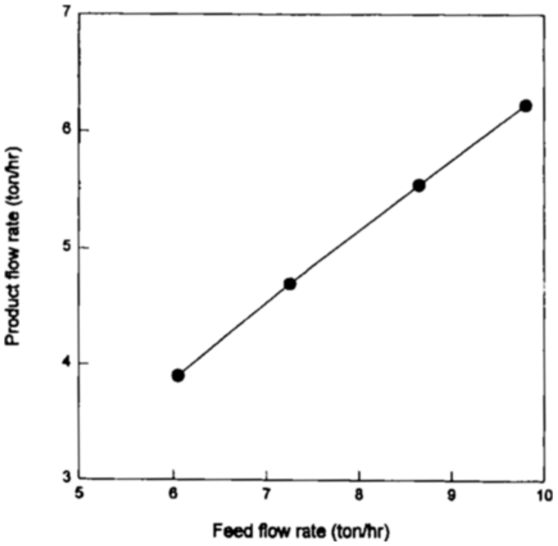

Fig. 7. Optimal production vs. feed change in toluene column.

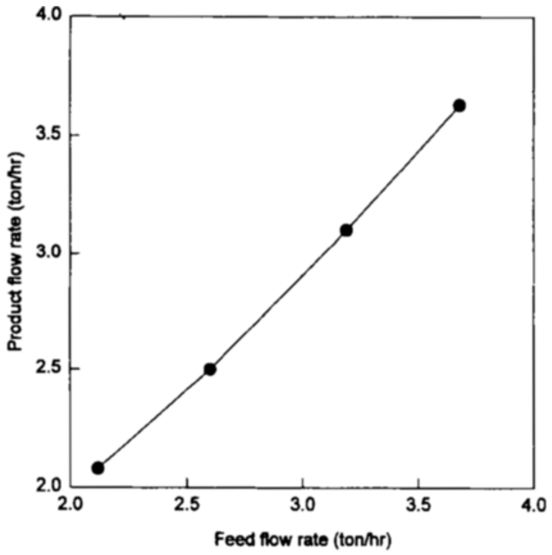

Fig. 8. Optimal production vs. feed change in xylene column.

xylene column is about 155 °C which is relatively lower than that of the feed.

In the operation, energy is consumed mainly by cooling water and steam. The reboiler and condenser duties are important variables in the feedforward control and optimization of the fractionation unit. Table 4 shows the relation between condenser and reboiler heat duties and feed load.

The optimal operating conditions for the fractionation unit were obtained based on the objective functions and constraints described before.

Figs. 6, 7 and 8 show results of optimization calculation for benzene, toluene and xylene column respectively. These results show optimal production rates for various feed changes with the feed compositions fixed. From these figures we can find optimal production rates with change of feed rates while maintaining the product purity as desired level. We can also affirm the fact that the column will produce the product proportional to the feed rate if we want to get the constant product purity in spite of the feed change in the column. Finally, in Figs. 9, 10 and 11, we can see that the optimum reflux ratio prevents energy costs from being needlessly expensive while keeping the product purity for various overhead production change in benzene, toluene and xylene columns. For xylene column we can see the decreasing reflux ratio although the product flow rate increases as shown in Fig. 11. From the fact we can see the reflux ratio has little effect on the product purity for xylene column as shown in Fig. 4.

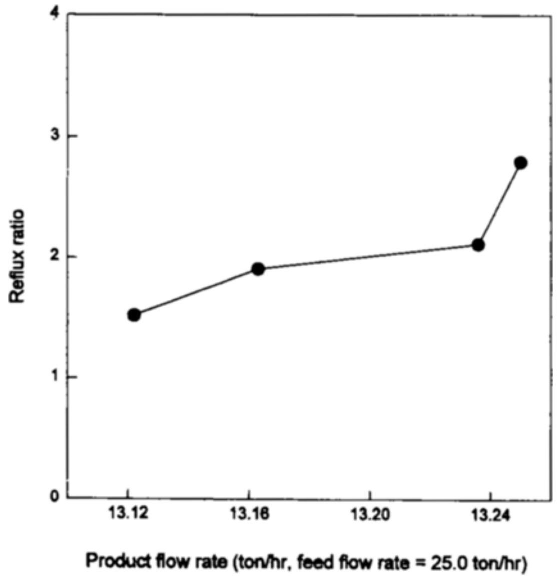

Fig. 9. Optimal reflux ratio vs. overhead production change in benzene column.

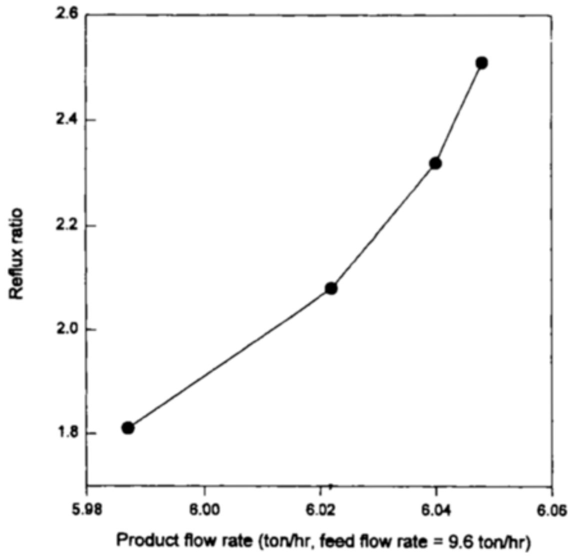

Fig. 10. Optimal reflux ratio vs. overhead production change in toluene column.

CONCLUSION

A steady-state optimization system for the industrial fractionation unit was developed based on modeling and simu-

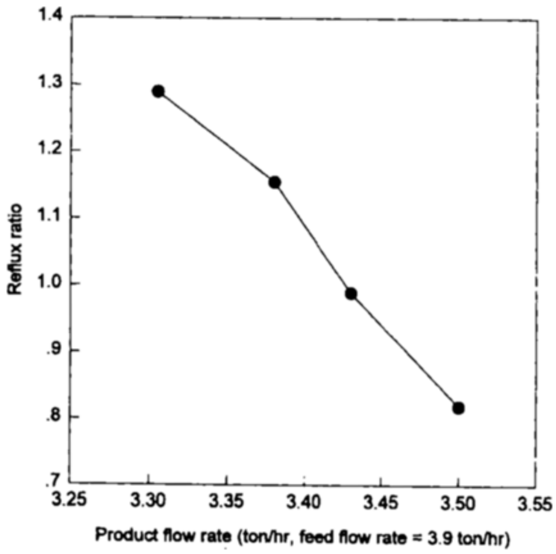

Fig. 11. Optimal reflux ratio vs. overhead production change in xylene column.

lation. The well-known boiling point estimation method and various thermodynamic state equations with some modifications were employed. Results of modeling and simulation showed good agreement with actual plant operation data. Based on the results of modeling and simulation optimal operating conditions were investigated. In the optimization, SQP method was used and key variables were incorporated in the objective functions. Optimal relations between production rates and feed rates were obtained and optimal reflux ratios were given as functions of required production rates. Extension of the present work to other BTX units are planned.

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NOMENCLATURE

$\mathbf{A}$: Jacobian matrix of constraints
A : coefficient for the SRK equation, $A=\sum_{i=1}^{c}\sum_{j=1}^{c} y_i y_j A_{ij}$ or $\sum_{i=1}^{c}\sum_{j=1}^{c} x_i x_j A_{ij}$ where $A_{ij}=\sqrt{A_i A_j}$
a_i : coefficient for the SRK equation, $a_i=(1+m_i(1-\sqrt{T_{r_i}}))^2$
A_i : coefficient for the SRK equation, $A_i=0.42747\ a_i \frac{P_{r_i}}{T_{r_i}}$
$\mathbf{B}$: approximation to the Hessian matrix used in sequential quadratic programming
B : coefficient for the SRK equation, $B=\sum_{i=1}^{c} y_i B_i$ or $\sum_{i=1}^{c} x_i B_i$
B_i : coefficient for the SRK equation, $B_i=0.08664 \frac{P_{r_i}}{T_{r_i}}$
D : product output
E_i : stage efficiency
F, F_j : feed flow rate, feed flow rate at stage j
$f(\mathbf{x})$: objective function
$g_j(\mathbf{x})$: inequality constraint
$\hat{\mathbf{H}}$: modified Hessian matrix
$(\hat{\mathbf{H}})^{-1}$: inverse Hessian matrix
$h_j(\mathbf{x})$: equality constraint
$\hat{h}(\mathbf{x}^k)$: vector of equality constraints
H_{Fj} : molar enthalpy of a feed
H_{Lj} : molar enthalpy of liquid phase
H_{Vj} : molar enthalpy of vapor phase
$\mathbf{I}$: identity matrix
$K_{i,j}$: equilibrium constant, K-value
L : Lagrangian
L_j : internal total liquid rate
m_i : coefficient for the SRK equation, $m_i=0.480+1.574w_i$ $0.176w_i^2$
P : penalty function
Q_j : heat duty
r : penalty function weighting coefficient
R_{max} : maximum reflux ratio
R_{min} : minimum reflux ratio
L/D : reflux ratio
$\mathbf{s}$: search direction
S_C : condensing cost in condenser
S_D : selling price
S_H : heating cost
S_F : feed cost
T_j : stage temperature
$\mathbf{u}$: vector of Lagrange multipliers
U_j : liquid sidecut
V_j : interval total vapor rate
V_S : steam flow going into reboiler
W_j : vapor sidecut
x_D : composition of overhead product
$x_{i,j}$: liquid composition
$y_{i,j}$: vapor composition
Z : compressibility factor
$z_{i,j}$: feed composition

Greek Letters

∇ : gradient operator ("del")
Δ : difference in general
ε : convergence criterion
λ : distance moved along a search vector (step length)
$\hat{\psi}$: fugacity coefficient

Superscripts

k : stage in search
T : transpose

Subscripts

i : component
j : stage

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