Control and Optimization of Aromatic Compounds in Multivariable Distillation Column

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Product separations in petroleum refineries depend significantly on distillation process, which is known to be challenging to be optimally managed, especially when multiple products with variety of purity requirements are involved due to nonlinear dynamics and high degree of process interactions. In this paper, control and optimization aspects of a multivariable distillation process are discussed. A mathematical model of the system is simulated in MATLAB programming environment, and analyses of process behavior and control performances are carried out. The controllers are tuned using conventional Ziegler-Nichols method and L-V control configuration was adopted. The results on disturbance rejection and set point tracking capabilities, in order to maintain the purity of benzene in the distillate above 98.5 % are discussed. Based on these insights, the optimum operating conditions were determined, which serves as a good starting point for further works in addressing variety of problems related to process operations.

1. Introduction

Distillation is considered an omnipresent and important separation method in petroleum refineries and chemical industries that is used in preliminary of final product purifications. Despite this widespread use, distillation is known to be heavily energy consuming process (Mahdi et al., 2015; Porru et al., 2013), and it is reported that nearly 60 % of the energy consumed in petrochemical and refining plants is associated with distillation processes (Mishra, 2011). Also, more than 50 % of plant operating cost is generated by distillation (van Diggelen et al., 2009). As such, it is important to thoroughly understand the process so that appropriate measures can be adopted to reduce energy consumption while maintaining product and profitability specifications (Khodadoost and Sadeghi, 2011). This demands good process control, majority of which can be addressed using PID controllers, with some specific cases demanding more advanced control algorithms. Based on a survey conducted by Kano and Ogawa (2010) the ratio of controllers used in the industry are estimated to be 100:10:1, showing the widespread use of PID control in relation to conventional advanced control, and model predictive control and 80 % of the PID control loops are successfully tuned.

The control of multivariable distillation processes is generally intricate due to their highly nonlinear characteristics, interactions between multiple inputs and outputs, process constraints and disturbances during operation (Xiong et al., 2014). Issues associated with nonlinear process characteristics are more intense in cases involving high purity products requirements. Depending of the nature of the plant and its location, variety of disturbances either due to interactions between process streams, upsets of utilities, or environmental factors. These difficulties pose numerous challenging control problems and have attracted the interest of research communities.

This paper discusses the multivariable control issues in an aromatic distillation process. The dynamic response and control strategies are investigated and optimum operating conditions are determined based on the purity requirement and energy consumption constraints. The model simulated in MATLAB programming environment.

2. Modelling and control

2.1 Process description

The schematic diagram of the BTX (benzene, toluene, xylene) multivariable distillation process used as a case study is shown in Figure 1 below. The feed enter the column in saturated liquid form onto the tray N_f. Benzene composition is specified to be in excess of 98.53 % in the overhead less than 3.37 % at the bottom product stream. Total condenser is used in the overhead and the operation data for all main streams are listed in Table1.
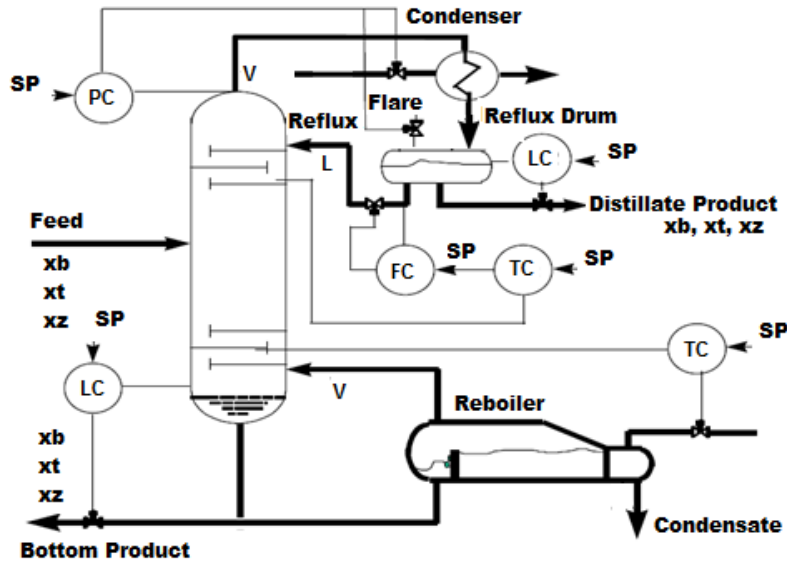

Figure1: Multi-component distillation column with proposed control structures

Table 1: The operation data for all main streams

External stream data	Feed	Top product	Bottom product
Stage number	6	1	10
Flow rate (kmol/min).	8	3.5	4.5
Temperature (K).	379.1	336.1	427.5
Pressure (atm).	1	1	1
Benzene (mol %).	45	98. 528	3.367
Toluene (mol %).	20	1.432	66.888
Xylene (mol %).	35	0.040	29.745
Reflux ratio	3.0		
Condenser duty (kJ/min)	363,385.491		
Reboiler duty (kJ/min)	367,226.574		

2.2 Mathematical modelling

The distillation system is modelled by partitioning it into five subsections, i.e., condenser tray, rectifying section, feed tray, stripping section, and reboiler tray. The following assumptions are made: (1) the vapour on the stage is in equilibrium with the liquid, (2) the liquid hold-up on each tray, condenser, and reboiler is constant at steady state and is perfectly mixed, (3) constant column pressure at 1 atm, (4) the hold-up in the vapour phase is neglected and only the liquid hold-up is considered, (5) the liquid and vapour molar flow rates through the stripping and rectifying sections are constant, and (6) the liquid composition and tray temperature are initialized and the equilibrium vapour composition can be calculated from constant relative volatility. The dynamic model is expressed by the following derivations:

The mass and energy balance in the condenser tray are given by

$$\frac{dM_1}{dt} = V_2 - (L_1 + D) ; \quad \frac{d(M_1 x_{1,j})}{dt} = V_2 y_{2,j} - (L_1 + D)x_{1,j} \tag{1}$$

$$\frac{d(M_1 H_1)}{dt} = V_2 H_{V,2} - (L_1 + D)H_{L,1} - Q_c \tag{2}$$

Here $x_{1,j}$ and $y_{i,j}$ are liquid and vapour mole fractions of benzene, toluene and xylene on the tray 1, D is the top product molar flow rate, L_1 is the liquid reflux flow rate, M_1 is the liquid hold-up in reflux drum, V_2 is the vapour molar flow rate comes on, H_L and H_V are liquid and vapour enthalpies, and Q_C is the condenser duty.

The mass and energy balance in the rectifying and stripping sections are given by

$$\frac{dM_i}{dt} = V_{i+1} - V_i + L_{i-1} - L_i \; ; \; \frac{d(M_i x_{i,j})}{dt} = V_{i+1,j}\, y_{i+1,j} - V_i\, y_{i,j} + L_{i-1,j} x_{i-1,j} - L_i\, x_{i,j} \tag{3}$$

$$\frac{d(M_i H_i)}{dt} = V_{i+1} H_{V,i+1} - V_i H_{V,i} + L_{i-1} H_{L,i-1} - L_i H_{L,i} \tag{4}$$

Since the liquid and vapour molar flow rates are assumed constant throughout each section, for liquid flow rates below the condenser and above the feed tray is represented by Eq. (5) and the liquid flow rate below the feed tray and above reboiler tray is given by Eq(6) (Skogestad, 1997):

$$L_i = L_1 + \frac{M_i - M_{0,i}}{taul} + (V_{i+1} - V_{Nt})lambda \tag{5}$$

$$L_i = (L_i + F) + \frac{M_i - M_{0,i}}{taul} + (V_{i+1} - V_{Nt})lambda \tag{6}$$

Here $M_{o,I}$ is the normal liquid hold-up on tray i, *lambda* is the effect of vapour flow on liquid flow which assumed close to zero, *taul* is time constant for the liquid flow dynamics, N_t is the reboiler tray, and F is the feed flow which is entering the column at boiling point ($q=1$).

The mass and energy balance in the feed tray N_f are given by

$$\frac{dM_{Nf}}{dt} = F + V_{Nf+1} - V_{Nf} + L_{Nf-1} - L_{Nf}$$

$$\frac{d(M_{Nf} x_{Nf,j})}{dt} = Fx_{f,j} + V_{Nf+1}\, y_{Nf+1,j} - V_i y_{Nf,j} + L_{Nf-1} x_{Nf-1,j} - L_{Nf}\, x_{Nf,j} \tag{7}$$

$$\frac{d(M_{Nf} H_{Nf})}{dt} = FH_f + V_{Nf+1} H_{V,Nf+1} - V_{Nf} H_{V,Nf} + L_{Nf-1} H_{L,Nf-1} - L_{Nf} H_{L,Nf} \tag{8}$$

The mass and energy balance in the reboiler tray N_t are represented by the following equations

$$\frac{dM_{Nt}}{dt} = L_{Nt-1} - V_{Nt} - B \; ; \; \frac{d(M_{Nt} x_{Nt,j})}{dt} = L_{Nt-1} - V_{Nt}\, y_{Nt,j} - B\, x_{Nt,j} \tag{9}$$

$$\frac{d(M_{Nt} H_{Nt})}{dt} = L_{Nt-1} H_{L,Nt-1} - V_{Nt} H_{V,Nt} - B H_{L,Nt} + Q_R \tag{10}$$

Here B is the bottom product flow rate and Q_R is the reboiler duty. The vapour-liquid equilibrium for multicomponent is calculate using the Eq (11) below (Halvorsen and Skogestad, 2003).

$$y_{i,j} = \frac{\alpha_j x_{i,j}}{\sum \alpha_j x_{i,j}} \tag{11}$$

Here α_j is the constant relative volatility of benzene, toluene, and xylene. Their values are 2.34, 1, and 0.44. The liquid and vapour enthalpies moving across the trays are calculated through thermodynamic rules as illustrated in Eqs(12) and (13).

$$H_{L,i} = \Sigma(Mwt_j x_{i,j} Cp_{L,i})\Delta T \tag{12}$$

$$H_{V,i} = \Sigma(Mwt_j \, y_{i,j} Cp_{V,i})\Delta T + \Sigma(Mwt_j \, y_{i,j})\lambda) \tag{13}$$

where Cp_L and Cp_V are the heat capacity of the components in liquid and vapour phase, Mwt_j is the molecular weight, ΔT is the difference between the standard and tray temperature, and λ is the latent heat of vaporization.

2.3 Control strategy

In general, there are several control configurations typically used for distillation process including L-V, D-B, D-V, L-B, and (L/D) (V/B) schemes (Skogestad, 1997). The choice is subject to the operating conditions and the nature of the processes, the more common of which is the L-V configuration that has been considered as almost a default. So, the L-V configuration which is the most common configuration used in the real plant (Skogestad and Morari, 1988) is also adopted for this study. The scheme is also noted for the ability to minimize the effect of process interactions (Sneesby et al., 1999).

The PID controller, which considers the present, past, and future errors is used, and is represented by Eq. (14) below (Das et al., 2012).

$$u(t) = K_c \left(e(t) + \frac{1}{T_i} \int_0^t e(t)*dt + T_d \frac{de(t)}{dt} \right) \tag{14}$$

Here $e(t)$ is the error of the process variable and its set-point value, K_c is proportional time constant which acts on the present value of the error, T_i is the integral time constant that represents an average of past errors, and T_d is the derivative time constant which takes into considerations the prediction of future errors. Ziegler-Nichols closed-loop method procedure is used to determine the ultimate of a proportional controller gain and period of oscillation of the loop.

3. Results and discussion

3.1 Optimization operation point

The process is optimized while maintaining some specified conditions and even when the process is subjected to disturbances. The optimal operation of the column should maximize the profit and minimize the cost function $(-J)$. The profit function (J) is represented as in Eq. (15) (Engelien et al., 2003),

$$J = D - w_r Q_r \tag{15}$$

where D is the top product flow rate (kmol/min), w_r is the relative energy cost (0.6488 kmol/kJ), and Q_r is the reboiler duty (kJ/min).

The purity and impurity of the top product are specified as operational constraints. So, the optimal operating points for the most important disturbances and implementation error for product purity are solved to identify the optimal cost for each case. According to the L-V configuration, the top reflux flow-rate L and bottom boil-up flow-rate V are used to adjust the control variables, which are the purity of the top product and the impurity of the bottom products.

Table 2: Optimal operating point for multivariable distillation column distillation

	xD mol%	xB mol%	D kmol/min	B kmol/min	L kmol/min	V kmol/min	L/D	Qr kJ/min	J kmol/min
Nominal	0.9853	0.0337	3.5	4.5	10.5	14	3.00	367,226.6	54.362
F + 20%	0.9853	0.0337	4.2	5.4	12.6229	16.823	3.00	395,292.2	65.726
F - 20%	0.9853	0.0337	2.8	3.6	8.4153	11.2153	3.00	339,326.6	42.998
xf =0.5	0.9853	0.0337	3.92	4.08	8.789247	12.710	2.242	354,539.6	61.505
xf =0.4	0.9853	0.0337	3.08	4.92	12.2489	15.3286	3.978	381,959	47.198
qf=0.9	0.9853	0.0337	3.5	4.5	11.3191	14.019	3.234	366,926.1	54.366
xD=0.99	0.99	0.03	3.5	4.5	11.7317	15.2317	3.352	379,618.2	54.228

To maintain the column inventories, i.e., the liquid level in the reflux drum and column base, the top flow-rate *D* and bottom flow-rate *B* are used. Since the column pressure is assumed constant, the cooling duty remains at constant flow-rate and reboiler heat duty is used to adjust the vapour flow-rate indirectly via steam flow (temperature at the column base). The results are shown in Table 2. The optimization results clearly show that the column is optimally operated and all operational constraints are satisfied.

3.2 Closed loop tuning

The control loop is aimed to maintain the purity of benzene in the top product and impurity in the bottom under acceptable specification while keeping the system operating in the safe zone by avoiding flooding and drought of the liquid in the reflux drum and reboiler. Step changes in manipulated variable (feed flow-rate) are used to obtain the dynamic response of the output (set-point) and the closed loop tuning using Ziegler-Nichols method is adopted. In this study, proportional and integral control (PI) controllers are used, and the control loops are tuned with step change in feed flow-rate 5 %. The closed-loops performances are analyzed by scrutinizing the response of the top and bottom composition, the reflux drum level, and reboiler level. The control gain values for P, PI, and PID are computed and listed in Table 3.

Table 3: Summary of controller parameters gains using Ziegler-Nichols method

controller	P	PI		PID		
	K_c	K_c	T_i (min)	K_c	T_i (min)	T_d (min)
Top product composition	20	18.182	1.833	23.529	1.10	0.275
Bottom product composition	40	36.364	2.083	47.059	1.25	0.3125
Reflux drum level	15	13.636	2.417	17.647	1.45	0.363
Reboiler level	5.5	5	2	6.471	1.2	0.3

3.3 Disturbance rejection

Dynamic simulation is a reliable method for evaluating control system design of a process (Yi and Luyben, 1995). Two steps up and down ±1 % and ±5 % in feed molar flow-rate are introduced, and the results showing the actions of the PI-controller rejecting the disturbances are as illustrated in Figure 2 (a, b, c, d, e, f). In all cases, successful results are obtained, and the process at maintained at a safe mode. The set-point of the top and bottom product of benzene are also tracked. The temperatures of the condenser and reboiler are kept close to its set-point and the level of reflux drum and reboiler are successfully maintained at acceptable range.
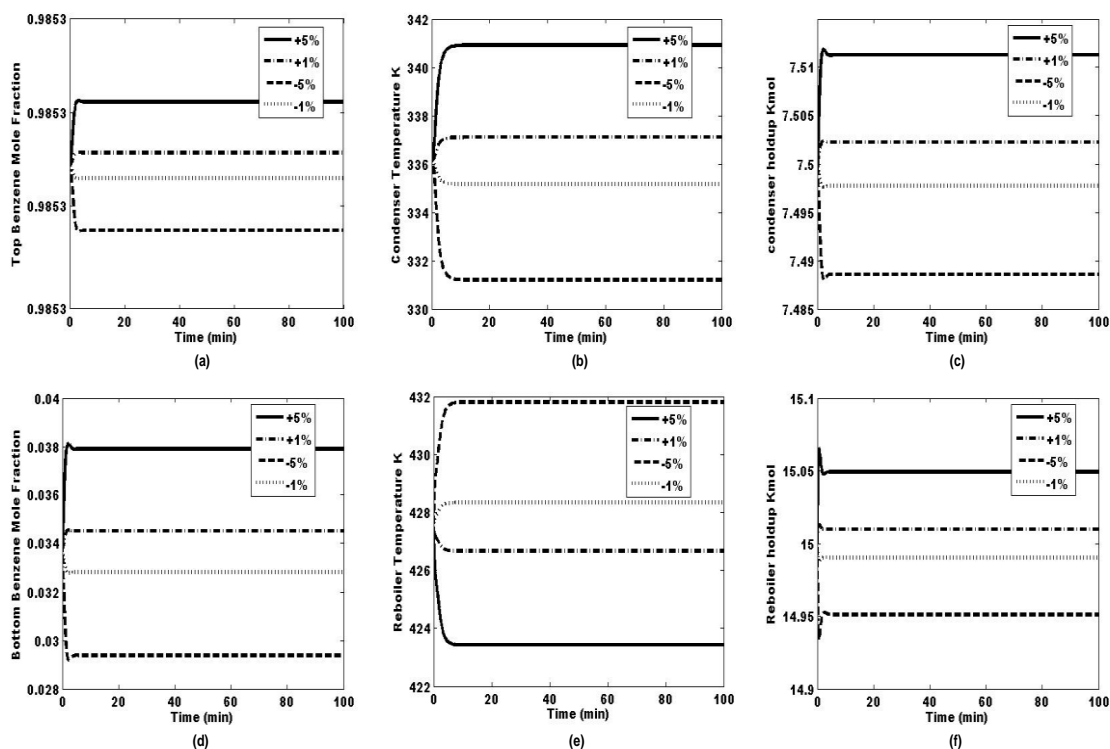

Figure 2: Dynamic response and feed flow-rate disturbance rejection with designed contol

4. Conclusion

The mathematical modelling and analyses of dynamic response of the distillation column based on nonlinear distillation process have been successfully implemented. The results of the optimal solution for both nominal case and disturbance rejection have demonstrated the capability of the proposed L-V control strategy in achieving the desired operation without violating the constraints and successfully eliminated the interactions between the variables. Also, the PI-controller have demonstrated the ability to reject persistent disturbance in feed flow rate in reasonably short times and tracked the set-point of the output products. The simulation results show the proposed control scheme keeps the energy consumption very close to the optimal point. This simulation test bed can now be used for further studies in distillation operations including detection of dynamic faults and implementation of risk-based operating schemes that are currently on-going.

Acknowledgment

References

Das S., Chakraborty A., Ray J.K., Bhattacharjee S., Neogi D.B., 2012, Study on Different Tuning Approach with Incorporation of Simulation Aspect for ZN (Ziegler-Nichols) Rules, International Journal of Scientific and Research Publications, 2, 58-64.

Engelien H.K., Larsson T., Skogestad S., 2003, Implementation of optimal operation for heat integrated distillation columns, Chemical Engineering Research and Design, 81, 277-281, DOI:10.1205/026387603762878755.

Halvorsen I.J., Skogestad S., 2003, Minimum energy consumption in multicomponent distillation. 3. More than three products and generalized Petlyuk arrangements, Industrial and Engineering Chemistry Research, 42, 616-629, DOI:10.1021/Ie0108651.

Kano M., Ogawa M., 2010, The state of the art in chemical process control in Japan: Good practice and questionnaire survey, Journal of Process Control, 20, 969-982.

Khodadoost M., Sadeghi J., 2011, Dynamic Simulation of Distillation Sequences in Dew Pointing Unit of South Pars Gas Refinery, Journal of Chemical and Petroleum Engineering, 45, 109-116.

Mahdi T., Ahmad A.,Nasef M.M., Ripin A., 2015, State-of-the-Art Technologies for Separation of Azeotropic Mixtures, Separation and Purification Reviews, 44, 308-330.

Mishra P, 2011, Modelling and control of binary distillation column using LabVIEW. Master dissertation, Delhi College of Engineering, Delhi, India.

Porru M., Alvarez J., Baratt R., 2013, Composition Estimator Design for Industrial Multicomponent Distillation Column, Chemical Engineering Transactions, 32, 1975-1980, DOI:10.3303/Cet1332330.

Skogestad S., 1997, Dynamics and control of distillation columns: A tutorial introduction, Chemical Engineering Research and Design, 75, 539-562, DOI:10.1205/026387697524092.

Skogestad S., Morari M., 1988, LV-control of a high-purity distillation column, Chemical Engineering Science, 43, 33-48.

Sneesby M.G.,Tade M.O., Smith T.N., 1999, Two-point control of a reactive distillation column for composition and conversion, Journal of Process Control, 9, 19-31.

Van Diggelen R.C.,Kiss A.A., Heemink A.W., 2009, Comparison of control strategies for dividing-wall columns, Industrial and Engineering Chemistry Research, 49, 288-307.

Xiong W., Chen L., Liu F., Xu B., 2014, Multiple Model Identification for a High Purity Distillation Column Process Based on EM Algorithm, Mathematical Problems in Engineering, 2014, 9, DOI:10.1155/2014/712682.

Yi C.K., Luyben W.L., 1995, Evaluation of Plant-Wide Control-Structures by Steady-State Disturbance Sensitivity Analysis, Industrial and Engineering Chemistry Research, 34, 2393-2405, DOI:10.1021/Ie00046a023.