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Procedia Engineering 148 (2016) 978 – 984

Procedia Engineering

www.elsevier.com/locate/procedia

4th International Conference on Process Engineering and Advanced Materials

Optimization and Dynamics of Distillation Column using Aspen Plus®

Syed A. Taqvi[a] , Lemma Dendena Tufa[a,]*, Shuhaimi Muhadizir[a]

[a]*Chemical Engineering Department, Universiti Teknologi Petronas, 32610 Bandar Seri Iskandar, Perak Darul Ridzuan, Malaysia*

Abstract

Ever increasing global energy demand necessitates the need to enhance energy generation and efficient utilization. As energy prices continue to rise, energy conservation is the prime concern for every industry. Distillation is probably the most studied unit operation in terms of optimization and control. Since distillation columns are major energy-intensive units in chemical plants and given the recent increase in fuel cost, the plant engineers are obliged to find better operating strategies and control systems. One of the significant sections that can be worked upon is finding the optimum feed tray locations of distillation columns. The energy consumptions during distillation can have a strong impact on overall profitability. Hence, the optimization of a column is aimed towards greater production and an increase in quality. Since a column is multivariable system, disturbance in any parameter can affect the overall performance as well as production loss. This paper shows how an acetone manufacturing process can be conveniently simulated first to get temperature, pressure and composition profile followed by application of optimization techniques to enhance performance. It was performed by the means of using a simulator Aspen Plus®. Rebolier heat duty (MW) and minimum reflux ratio were successfully optimized by manipulating feed stage location and number of stages respectively. It was observed that minimum reboiler duty is 40.8 MW when feed is at stage 10 resulting in 98% acetone as distillate.

Peer-review under responsibility of the organizing committee of ICPEAM 2016

Keywords: Distillation Simulation, Column Optimization, Dynamic modeling, Aspen Plus®, Aspen Dynamics®.

1. Introduction

Process industries, in pursuit of achieving their business objectives, given the continuously changing market dynamics and strong environment regulations in place, are designing plants for an optimum performance along with reduced risk of rework by employing simulation studies [1].

Simulation & control studies are widely in practice for batch and continuous chemical process operations for last two decades [2, 3]. In the last two decades there has been a remarkable increase in application of computational techniques which are readily available for engineers [4]. Owing to these advantages engineers can easily use more profound techniques of analysis and synthesis. There is a room of improvement in mathematical modeling but the dynamics of most systems can still be described effectively for engineering purpose [5]. Distillation column has been the subject of discussion for the last two decades in both the research and industrial arena for its modeling and simulation [6-12].

Optimization techniques have been applied to problems of industrial importance ever since the late 1940s. Distillation processes are most essential unit operations in chemical engineering. They are of significant importance as separation methods in

* Corresponding author. Tel.: +60-12 269 6816, Fax: +605-365-6176
E-mail address: lemma_dendena@petronas.com.my

1877-7058
Peer-review under responsibility of the organizing committee of ICPEAM 2016
doi:10.1016/j.proeng.2016.06.484

chemical and petroleum industries. Chemical and petroleum industries hold a significant share in the overall world economy. Distillation processes have huge maintenance and running cost that can be greater than the overall cost of many other processes. Therefore, there should be an effective a reliable control system for efficient and safe operation of a distillation column. It presents various challenging control problems. Distillation columns are highly multivariable and shows non-linear behaviour. Therefore, their control is not a trivial task [13].

Distillation design analysis comprises of detailed study of vapor-liquid equilibrium calculation in some case vapor-liquid-liquid (phase) equilibrium (VLLE) along with tray to tray component balances when discussing about digital computations [14-16]. Dynamic simulations of distillation columns are extensively in practice to develop effective control strategies. In the present study, steady-state simulations are being performed using Aspen Plus® followed by Aspen Dynamics® simulation, licensed software of Aspen Tech®. Aspen Dynamics® is a dynamic simulator commonly used to investigate the dynamics and control of continuous processes around some steady-state design operating point. Aspen Plus enhances the process of building and running the process simulation by adding a comprehensive system of online process modelling [2,5,15,17,18].

Aspen Plus and Aspen Dynamics developed a very sophisticated simulation that involves multiple complex steps and scripts in a very lengthy design and analysis procedure. Researchers have combined the steady-state simulator Aspen Plus and Dynamics simulator Aspen Dynamics for the simulation of control strategies [13,19, 20]. One can easily predict the behavior of any process by using fundamental and engineering relationship such as mass and energy balance, phase and chemical equilibrium. Process simulation has the ability to run different cases like “what if” analysis, sensitivity analysis and to do optimization runs. Simulation can design optimized plants as well as can also increase the profitability of existing plant by doing number of runs.

Nomenclature

V	Vapor boilup
R	Reflux flow
D	Distillate flow rate
L	Liquid flow rate
B	Bottom flow rate
α	Relative volatility
y	Vapor composition
x	Liquid composition
M	Holdups (liquid/Vapor)
h	Enthalpy (energy/mole)
N_F	Feed stage

2. Steady-State Continuous Process Modeling Setup

Acetone is used as solvent for biological sensitive process as well as in pharmaceutical formulation. The fully instrumented control Distillation Column is a distillation column situated in Block III University Technology PETRONAS that can be self-sufficiently run using mixture of Isopropanol (IPA) and Acetone. The First Step is to set up a simulation in Aspen Plus® that has the required pieces of equipment to size the column and auxiliary equipment of desired capacity. It should be noted that in Aspen Plus flow sheet must be a continuous process with the feed and product stream. Systematic and realistic modeling has been done to develop an understanding about distillation column parameters variation to maintain product quality. The fictitious and large feed consisting of binary mixture IPA and Acetone at a known composition (mixture 30% acetone composition) is pumped from the feed tank via Heat Recovery Exchanger into the distillation column at a desired temperature and at a desired feed point as mentioned in figure 1. The following Unit Operation Block data has been used to simulate column as mentioned in Table 1.

Pilot scale distillation column block III UTP, is used to make a case study in simulation. Column comprises of 15- bubble cap tray with the size of DN 150x5.5 m (H) with approx. 35cm tray spacing. Weir height is assumed to be0.0025 m and tray pressure drop is 0.01 bar per tray. The basic Aspen Plus® RADFRAC has been selected that incorporates implicitly a condenser and a reboiler. RADFRAC calculates the T, P, x, y, V and L on every stage. It estimates the temperature profile based on bubble and dew point temperatures of feed. RADFRAC columns allows to be operated in rating or design mode. The feed conditions and other parameters are mentioned in Table 2 below. The top stage is stage 2 and the bottom one is stage 14 with the condenser and reboiler as stage 1 and 15 respectively. Total condenser has been selected to get liquid from condenser.

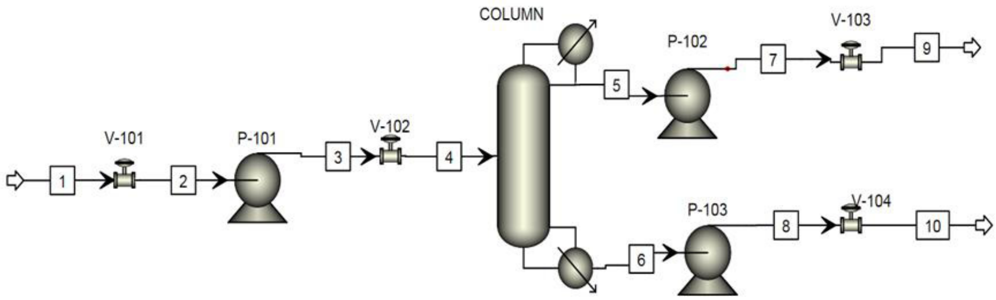

Fig.1. Aspen Plus® Steady-State Simulation

Table 1: Column/Reboiler Specification (Reference to UTP Block III distillation Column)

Distillation Column (T-100)			
Specifications	Details	Specifications	Details
Column Height	150 mm	Type of Tray	Bubble Cap Tray
Colum Diameter	5.5 m	Tray Spacing	Approx. 35 cm
No. of Trays	15-plates	Material of Construction	Stainless Steel
Feed Stage	variable	Other specifications	2 tray per section

Table 2: Feed Condition and other Specifications (Reference to UTP Block III distillation Column)

Specifications	Feed	Specifications	Feed
Temperature [C]	30.0	Reflux Ratio [molar]	3.0
Pressure [kPa]	105.6	Distillate Rate [kmole/hr]	1080
Molar Flow [kmole/h]	3600.0	Condenser Pressure [kpa]	101.3
Acetone mole fraction	0.3	Reboiler Pressure [kpa]	105.7
2-Propanol mole fraction	0.7		

2.1. Thermodynamic Property Package

The choice of appropriate thermodynamic model and the accuracy of parameters are crucial for the reliability of design. The Nonrandom Two-Liquid (NRTL) Model equation of state physical has been selected as property package (base method) in Aspen HYSYS steady-state Simulation. NRTL model is generally suggested for highly non-ideal chemical systems and can be used for both VLE and LLE applications [18, 21].

2.2. Mathematical Model

A binary system (two components) with constant relative volatility throughout the column and theoretical (100 percent efficient) trays, i.e., the vapor leaving the tray is in equilibrium with the liquid on the tray has been assumed. This means the simple vapor-liquid equilibrium relationship can be used [5];

$$y_n = \frac{\alpha x_n}{(1+(\alpha-1)x_n} \tag{1}$$

A single feed stream is fed as saturated liquid at its bubble point onto the tray N. Feed flow rate is F(mole/min) and composition is Z(mole fraction of more volatile component). The overhead vapor are totally condensed in a condenser and flows into reflux drum, whose holdup is M_D (moles). The contents of the drum are assumed to be perfectly mixed with composition x_D. The liquid in the drum is at its bubble point. Reflux is pumped back to the top tray (N_T) of the column at rate R. Overhead distillate product is removed at rate D. At the base of the column, liquid bottoms product is removed at a rate B and with a composition x_B. Vapor boilup is generated in a thermosiphon reboiler at a rate V We will assume that the liquids in the reboiler and in the base of the column are perfectly mixed together and have the same composition x_B and total holdup M_B (moles).

Condenser and Reflux Drum

Component continuity (more volatile component):

$$\frac{d(M_D x_D)}{dt} = V y_N - (R + D) x_D \quad (2)$$

Reboiler and Column Base:

Total Continuity:

$$\frac{dM_B}{dt} = L_1 - V - D \quad (3)$$

Component Continuity:

$$\frac{d(M_B x_B)}{dt} = L_1 x_1 - V y_B - B x_B \quad (4)$$

The steady state operation of each module comprises of following equations, commonly referred to as the MESH equations. [MESH = material balance equations, efficiency relations, summation equation, and heat (enthalpy) balance equations].

Material balance equation:

$$L_{i+1} + V_{i-1} - L_i - V_i = 0 \quad (5)$$

Stage efficiency relations:

$$y_i - y_{i-1} = \eta_{ij}[y_i^*(x_i, T_i, p_i) - y_{i-1}] \quad (6)$$

Where, $y_i = \frac{v_i}{V_i}$ and $x_i = \frac{l_i}{L_i}$

Summation equation:

$$L_i = \sum_{j=1}^{NC} l_{ij} \quad (7)$$

$$V_i = \sum_{j=1}^{NC} v_{ij} \quad (8)$$

Enthalpy balance equation:

$$L_{i+1} h_{i+1} + V_{i-1} h_{i-1} - L_i h_i - V_i h_i = 0 \quad (9)$$

2.3. Assumptions

The distillation column consists of non-ideal column with following assumptions;

- The Liquid on the tray is perfectly mixed and incompressible.
- Tray vapor holdups are negligible.
- Dynamics of the condenser and the reboiler is neglected.
- Vapor and liquid are in thermal equilibrium (same temperatures) but not in phase equilibrium.
- The column is assumed to be completely insulated.

2.4. Column Optimization Parameters

Energy reduction in chemical processes is essential for energy optimization and cost effective production. However, distillation is highly energy intensive and can consume nine-tenths of the total energy in a typical chemical or petrochemical process. In most distillation column the major operating cost is reboiler energy consumption. In simulation a design specification has been used to maintain the top and bottom composition of column to achieve maximum purity. This can be done by using optimization approach for column feed location, minim no. of trays and minimum reflux ratio. Selecting optimum feed location is critical to maximizing distillation column performance. Improper feed location of a distillation column can downgrade column performance; the degree of separation is decreased at the same reflux/boil up ratio or the higher reflux/boil up ratio is required to maintain the degree of separation [21]. The objective is to minimize the reboiler heat duty which accounts for a major portion of operating costs. The optimization problem is therefore given by,

Objective function 1:

$$Minimize\ Q_B$$

Subject to:

$$8 \le N_F \le 12$$
$$L_N, V_N, T_N \ge 0$$
$$Q_B, Q_C, D, B \ge 0$$
$$N = 15$$
$$x_F = 0.3$$
$$x_D = 0.98, \quad y_D = 0$$
$$\Delta P_i = 0.01\ bar,\ 0 < n \le 15 \text{ (Integer)}$$
$$\mathrm{L/D} = 3.0$$
$$\mathrm{D} = 1080 \frac{\mathrm{kmole}}{\mathrm{hr}}$$
$$\mathrm{P_1} = 101.3\ \mathrm{kpa}, \quad \mathrm{P_{15}} = 105.7\ \mathrm{kpa}$$

Objective function 2:

$$Minimize\ R$$

Subject to:

$$15 \le N \le 45$$
$$L_N, V_N, T_N \ge 0,$$
$$Q_B, Q_C, D, B \ge 0$$
$$N_F = 2N/3$$
$$x_F = 0.3$$
$$x_D = 0.98, \quad y_D = 0$$
$$\Delta P_i = 0.01\ bar,\ 0 < n \le 15 \text{ (Integer)}$$
$$\mathrm{L/D} = 3.0$$
$$\mathrm{D} = 1080 \frac{\mathrm{kmole}}{\mathrm{hr}}$$
$$\mathrm{P_1} = 101.3\ \mathrm{kpa}, \quad \mathrm{P_{15}} = 105.7\ \mathrm{kpa}$$

2.5. Aspen Dynamics

For the development of control strategy, it requires the conversion of steady state model in a dynamic one. The model developed in Aspen Plus is exported to Pressure-Driven simulation in Aspen Dynamics. Before exporting to Aspen dynamics, the size and the initial specification each equipment must be identified that includes (valve pressure drops, pumps suction or discharge pressure etc. In Aspen Plus column dynamics the reflux drum is size to have a diameter of 4.08 m and length is 8.16 m and the sump is sized to have a diameter of 5.08 m and height is 10.16 m. In column hydraulics, column diameter, tray spacing and weir height have been mentioned to complete the geometry of distillation column. It should be noted that pumps are not used to on the streams whose flow rates will be set to zero because error message will appear in Aspen Dynamics when the flow through a pump is zero. At this stage the file is now ready to be checked as a realistic pressure-driven dynamics simulation can be studied. This can be done by clicking pressure checker that either this file ready to move to Aspen Dynamics or not. In case of correctly defined plumbing, the file is ready to export into Aspen Dynamics to generate "dynf" extension file.

2.6. Initial Setup of Aspen Dynamics and Control Structure

After successfully export of file "dynf" and when it is opened in Aspen Dynamics, the first thing is to check is either integrator is running okay. There is common error message which is in practice can be noted as "Failure to initialization". This is because of plumbing error, so there must be some correction in Aspen Plus® Steady State to configure the control structures appropriately. A larger diameter column with 15 trays would take some time to send vapor at the top of the column. Once the vapor gets to the top of the upper column, it is condensed and liquid begin to fill the reflux drum. When the sufficient liquid is built up to satisfy pump NPSH requirement, then the liquid in the reflux drum is maintained at low level. The initial flow sheet that opens up in Aspen Dynamics is shown in Fig. 2. A default controller has been automatically installed with the closed loop process flow diagram i.e. pressure controller at the condenser, in control configuration panel it can be seen that the default for the pressure ranges are from (0-2 bar) and this controller is maintaining the controller pressure by manipulating the condenser heat removal (direct Qc) The Aspen Plus default tuning parameter are used (K_c =20 and τ_I= 12 min).

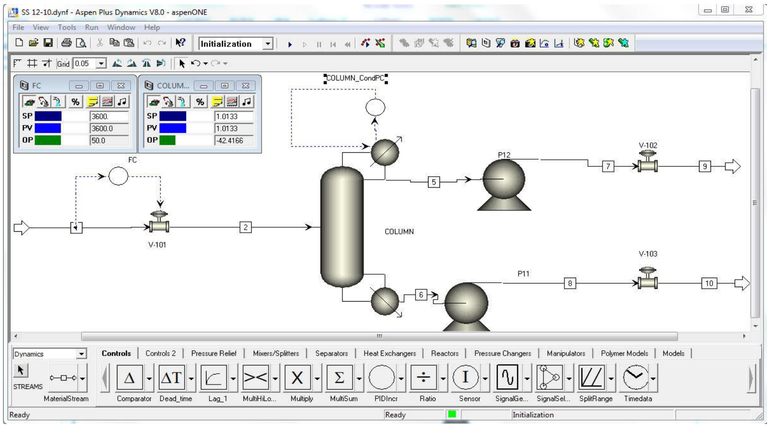

Fig. 2. Initial Aspen Dynamics flowsheet after exporting

3. Results and Discussions

3.1. Steady State Simulation

First Step of this study was the analysis of a given binary mixture system, with a defined physical property package. Aspen physical property system has a large no. of built-in binary parameter for different models. The column specification diagram i.e. temperature, pressure, composition can easily be generated in Aspen with the calculation of phase equilibrium relationship that are all hidden is Aspen data bank. The column temperature and composition profile can be obtained by selecting block column and plot the profile as mentioned in Figure 3. The composition of Acetone can be noted as 97% pure at top of the column at reflux ratio 3 molar.

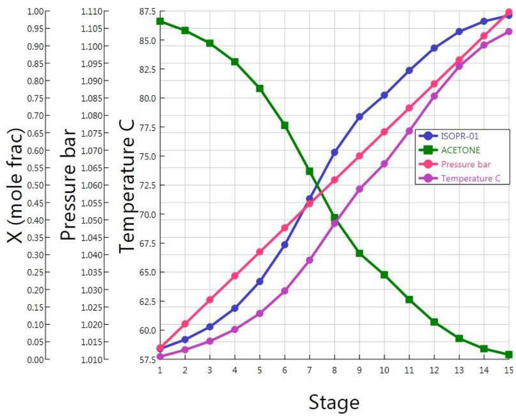

Fig.3: Temperature, pressure and composition profile of column

3.2. Optimum Feed Tray and Minimum Conditions

Once the pressure, temperature and composition profile has been determined along with mole purity has been set to the desired value, so we can find the optimum feed tray. In addition, the minimum reflux ratio and the minimum no. of stages can also be determined to run the column at optimal conditions. The Simulation is run at fixed top and bottom composition to get the optimum feed tray.

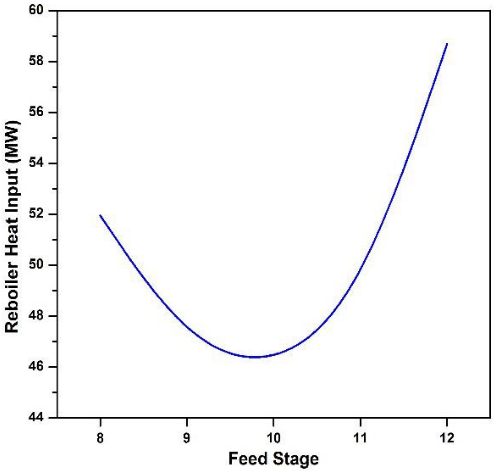

Fig. 4. Effect of Feed Stage on Reboiler Heat Input

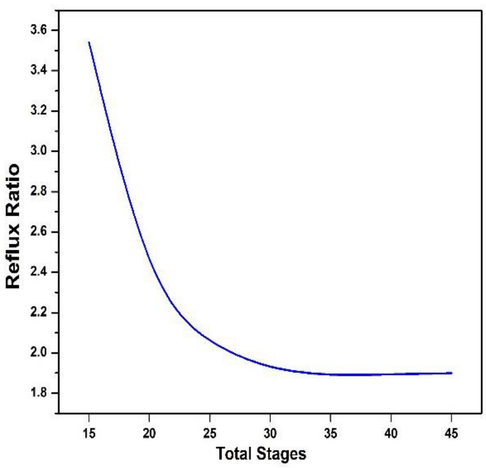

Fig. 5. Effect of Total Stages on Minimum Reflux ratio

As shown in Fig. 4, It can be seen that feed on stage 10 gives the minimum energy consumption i.e. 40.8 MW to achieve 98% Acetone as distillate. The simulation can be used to find the minimum reflux ratio by increasing the no. of stages until there is no further reduction in reflux ratio as shown in fig. 5. As product purities are kept constant. It is assumed that the feed stage is a fixed ratio of total no. of stages.

4. Conclusion

This article presents the optimization and dynamics of distillation column for acetone production unit. The design flow sheet is simulated using NRTL thermodynamic model which describes vapor liquid equilibrium data appropriately. It can be witnessed that Aspen Plus and Aspen Dynamics is a comprehensive tool which can be used to optimize the column and can be used to develop different control strategies. An appropriate control structure can be modeled from Aspen Dynamics control model library to develop a realistic scheme that will be helpful to understand physical reality.

References

[1] H. Kister, Distillation operation,1990
[2] W. L. Luyben, Aspen Dynamics simulation of a middle-vessel batch distillation process, Journal of Process Control. 33 (2015) 49-59.
[3] W. L. Luyben, Distillation design and control using Aspen simulation: John Wiley & Sons, 2013.
[4] A.C. Dimian, C. S. Bildea, and A. A. Kiss, Integrated design and simulation of chemical processes vol. 35: Elsevier, 2014.
[5] W. L. Luyben, Process modeling, simulation and control for chemical engineers: McGraw-Hill Higher Education, 1989.
[6] D. Gil, J. M. Gomez, and G. Rodriguez, Control of an extractive distillation process to dehydrate ethanol using glycerol as entrainer, Computers & Chemical Engineering. 39 (2012) 129-142.
[7] S. Hurowitz, J. Anderson, M. Duvall, and J. B. Riggs, Distillation control configuration selection, Journal of Process Control. 13 (2003) 357-362.
[8] M. W. Maciel and R. Brito, Evaluation of the dynamic behavior of an extractive distillation column for dehydration of aqueous ethanol mixtures, Computers & chemical engineering. 19 (1995) 405-408.
[9] Olsen, G. O. Endrestøl, and T. Sira, A rigorous and efficient distillation column model for engineering and training simulators, Computers & chemical engineering. 21 (1997) S193-S198.
[10] R. Ross, J. Perkins, E. Pistikopoulos, G. Koot, and J. Van Schijndel, Optimal design and control of a high-purity industrial distillation system, Computers & Chemical Engineering. 25 (2001) 141-150.
[11] M. Rovaglio, E. Ranzi, G. Biardi, and T. Faravelli, Rigorous dynamics and control of continuous distillation systems—simulation and experimental results, Computers & Chemical Engineering. 14 (1990) 871-887.
[12] F. G. Shinskey, Process control systems: application, design and tuning: McGraw-Hill, Inc., 1990.
[13] Guy, Dynamic modeling of continuous-distillation and emergency systems, Chemical Engineering. 90 (1983) 65-69.
[14] P. S. Fruehauf and D. P. Mahoney, Distillation column control design using steady state models: Usefulness and limitations, ISA Transactions. 32 (1993) 157-175.
[15] W. L. Luyben, Control of a multiunit heterogeneous azeotropic distillation process, Aiche Journal. 52 (2006) 623-637.
[16] Kitterman, Tower internals and accessories, in Congresso Brasileiro de Petroquimica Rio de Janeiro1976
[17] W. L. Luyben, Practical distillation control: Springer Science & Business Media, 2012.
[18] W. L. Luyben and I.-L. Chien, Design and control of distillation systems for separating azeotropes: John Wiley & Sons, 2011.
[19] J.-Y. Yao, S.-Y. Lin, and I.-L. Chien, Operation and control of batch extractive distillation for the separation of mixtures with minimum-boiling azeotrope, Journal of the Chinese Institute of Chemical Engineers. 38 (2007) 371-383.
[20] H. J. Huang and I.-L. Chien, Choice of suitable entrainer in heteroazeotropic batch distillation system for acetic acid dehydration, Journal of the Chinese Institute of Chemical Engineers. 39 (2008) 503-517.
[21] J.-C. Lee, Y.-K. Yeo, K. H. Song, and I.-W. Kim, Operating strategies and optimum feed tray locations of the fractionation unit of btx plants for energy conservation, Korean Journal of Chemical Engineering. 18 (2001) 428-431.