Optimation Condition Operation of Distillation to produce 2-EHA using ChemSep Version 8.23

Abyadh Basyari Fahmi∗, Agung Sugiharto, Rois Fatoni
Department of Chemical Engineering, Faculty of Engineering, Universitas Muhammadiyah Surakarta, Surakarta, Indonesia Jl. A. Yani Tromol Pos 1 Pabelan Kartasura 57102 Telp 0271 717417
E-mail: ∗babyadh@rocketmail.com

Abstract. A new methodology for optimation column distillation process has been developed not only by manual calculation but recently technology take in the forward and improving of any simulator available to use. Sophisticated technology of simulator has been used for this optimisation as well as Aspen Hysys is available for obtaining the best way of production plant. Simulator use a variety of thermodynamics calculation to operate and it depends on the type of distillation, phase of the components and operation condition of the simulation. In this paper, a critical review of optimisation condition concern to utilize simulators capability including selection of thermodynamics property packages, test of several variable operation condition especially on the temperature and pressure also the combining and correction the value of the composition polymerization of acrylic acid. For future project commissioning of industrial plant make use of the simulator such as Aspen Hysys is highly recommend to hold significant potential and great promise for further evaluation, development and application.

1. Introduction
Acrylic acid is the raw material for the production of 2-Ethylhexyl Acrylate (2-EHA) which is reacted with 2-Ethylhexyl Alcohol. Acrylic acid can cause polymerization in the purification column of the 2-EHA production process. Therefore, the acrylic acid content in the purification column is kept as small as possible so that it does not evaporate at the top of the purification column even if using high temperature and have to keep it above the boiling point of water. If a large amount of acrylic acid evaporates and the water content above the purification column is insufficient, polymerize can form and it will interfere with the production process [3].

Acrylic acid is a water soluble compound. Acrylic acid will undergo a polymerization process at a relatively high temperature (turning into a dimer, trimer, tetramer, etc.). Acrylic acid polymers has possibility to occur rapidly when the water content decreases, so that polymerization can form in dry areas on the walls and in the distillation sky. So, boiling point is important in distillation column and the operating conditions are similar part of the production process. Because, by setting the right temperature and also the right time, polymerization can be minimized [4].

The operating conditions can affect the boiling point which is a combination of temperature and pressure. Thus, optimization of operating conditions is necessary to maximize production and efficiency. The lower amount of polymerization that occurs in the purification column, the purer the product will be [11].
There is an alternative for optimization in the distillation column by using ChemSep. ChemSep is one of the best simulators used to improve distillation units. Because in several existing studies ChemSep is widely used as a good simulator for distillation equipment because it can calculate thermodynamic mathematics highly accurate compared to actual results in the field [6]. The U.S. The Dept of Energy simulates more than 40,000 column distillations for its plant operations as well as in the refining section of its chemical industry using Chemsep V6.5. Development with simulators is used to improve the energy efficiency of the operating unit with the optimal use of temperature [14]. Chemsep uses commonly in many types of distillations such as in azeotropic distillation, simple distillation and column distillation [12].

Distillation process design in industrial practice is normally can be simulate by several iteration solution with input the design specification before simulate the operation. The simulation is usually required high skill to operate it by computing cause the requirement of input needly is normally not same by actual, eventhough the simulation is normally can guarantee to obtain the best result for economically / optimal design given [1]. Due to highly difficulty of using simulation, it becomes rarely user and expensive value to operate to the process. The successful of a simulation is based on the initial corrective input values [2].

Simulator software has variety function depend on the specifically, such as ChemSep Lite version is tactically used for interacting via CAPE-OPEN which has been established, validated and demonstrated for almost 15 years to solve calculation between material, energy and the data specification to be mathematical thermodynamics equation. The purpose of ChemSep is clearly simplify the flowsheets of i.e. simple distillation, stripper and absorber to optimize the necessitate component [7].

Recently, publications regarding the prevention of acrylic acid prevention in the production of 2-EHA are still used as alternatives. However, the optimization has never been carried out. Existing alternatives include: 1. Prevention of polymerization of acrylic acid can be accomplished by adding oxygen together with inhibitors such as hydroquinone and phenothiazine. The inhibitors feed from the top of the distillation and flows to the bottom of the distillation especially to the reboiler and also feed from the reboiler of distillation. So, inhibitor feed from 2 ways which are top side and bottom side. The research has the advantage of obtaining the optimal requirement of about 0.01 to 5% per bottom yield volume of the polymerization to bottom side [9].

A further alternative is to use a non-volatile inhibitor in the distillation column and a volatile inhibitor such as nitric oxide in the condenser to prevent unwanted premature acrylic acid polymer. Non-volatile inhibitor used to prevent acrylic acid state on the same phase and not evolve[10].

A modification alternative also being used with changing of the simple distillation to vacuum distillation which consider to try over the operating condition < 500 mmHg absolute pressure and the temperature of 50°C till 170°C can also be done to prevent polymerization. The study has the advantage of controlling acrylic acid polymers [11]. The last alternative also modification the equipment which is using distillation reactive batches and also amberlyst 70 catalyst in each package can be utilized on the industrial scale. In addition, decanters are also used for one of the water components in the distillation output after the condenser. This research has the advantage that acrylic acid can be converted by 80% caused acrylic acid is high solubility in water [8].

The fourth alternatives has been presented with the same drawback, namely the absence of a concentration of 2-EHA in accordance with the required market specification. Therefore, the researcher wants to try to remove acrylic acid polymers with optimal temperature, pressure and the combination to minimize acrylic acid polymerization also obtain the required 2-EHA as the market specification.
2. Methods

2.1. Selection of the Components

The data component of production 2-Ethylhexyl Acrylate has actually carried by actual data of
the plant. It has been provided that properties of the raw material is eventually same with the
simulator (acrylic acid and 2-ethylhexyl alcohol). Before input the data, unknown component
by ChemSep is hypothetically create manual as below:

(i) Open PCD manager
(ii) Add new then input the name component
(iii) Selected the matched “Check Essential data”
(iv) Fill the data as the standard
(v) If all is green OK then save as and ready to use in ChemSep.

Figure 1: Add new Component

In the PCD manager of ChemSep could be create or hypothesize new component based on the
several important requirement, such as below:

(i) CAS Number
(ii) Molecular weight
(iii) Critical point (Temperature, Pressuerr, Volume, Compressibility)
(iv) Boiling point
(v) Liquid molar volume at boiling point
(vi) Acentric factor

For the CAS number we can found it on the google searching cause it can be same for all
simulator using. Then input the components as below:

2.2. Selection of the type of Operation

Type of operation normally has many typical choice and function. But in this paper, it uses
simple distillation cause the actual plant also used the same as the simulate. In the selecting
the type of operation selection, accuracy is needed in accordance with the actual conditions at
the plant. Because, different types of operation will affect to the conditions and results of the
operations.
2.3. Selection of the Properties Termodynamics

Properties is a combination of a component list you defined in the components and navigate of the typically thermodynamic state configuration such as K-Value, EOS, Activity Coeff, etc. to obtain the result after calculate with thermodynamics method which based on industry specific property derivation formula such. In this paper used, NRTL cause it can be used for liquid liquid equilibrium phase (LLE) also.

Gamma-Phi is used for this research cause it used for calculated K-values an activity coefficient model for the liquid phase and an equation state for the vapor, so it can be combine with NRTL which only focused on the liquid vapor phase, and the formula is following as below:
\[ K_i = \frac{\gamma_i \cdot \varphi_i \cdot P_i}{\varphi v_i} \]  \hspace{1cm} (1)

Where: \( \gamma_i \) = Activity coefficient of component \( i \), \( \varphi_i \) = Disperse phase holdup fraction \( i \), \( P_i \) = Power input, \( v_i \) = Tray volume for interfacial mass transport. The K-values of Gamma-Phi is dealing with nonideal fluid mixtures and should not be selected for separations at high pressures. So it’s suitable for this research to used [5]. The NRTL equation proposed to used in the Vapor Liquid Equation (VLE) which consist on the ratio of the molar mass of the pure components. The formula of NRTL equation following as below (13):

\[
\ln \gamma_i = \frac{\sum_{j=1}^{n} \tau_{ij} x_j G_{ji}}{\sum_{k=1}^{n} x_k G_{ki}} + \sum_{j=1}^{n} \frac{x_j G_{ij}}{x_k G_{kj}} \left( \tau_{ij} - \frac{\sum_{m=1}^{n} \tau_{mj} x_m G_{mj}}{\sum_{k=1}^{n} x_k G_{kj}} \right) \]  \hspace{1cm} (2)

Where: \( \gamma_i \) = Activity coefficient of component \( i \), \( G_{ij} = \exp(-\tau_{ij} \alpha_{ij}) \),

\[
\tau_{ij} = \frac{a_{ij} + b_{ij} T}{RT} \]  \hspace{1cm} (3)

\( x_i \) = Mole fraction of component \( i \), \( T \) = Temperature (K), \( n \) = total number of components, \( a_{ij} \) = Non-temperature dependent energy Parameter between components \( I \) and \( j \) (Cal/gmol), \( b_{ij} \) = Temperature dependent energy parameter Between components \( i \) and \( j \) (Cal/gmol-k), \( a_{ij} \) = NTRL constant for binary \( a_{ij} = a_{ij} \) For all binaries.

2.4. Selection of the Feed
In the feed table has several data to input such as Temperature, Pressure and the composition of the operation. Feed table used widely for trial and error from the actual data and compare with the actual to get the best result.

2.5. Selection of the Specifications
In the specifications line shall be input the pressure of condenser, heater/coolers energy, efficiency of the column and the last is column specs include the condenser & reboiler specification.

Specification of table consist of many important variable such as analysis of ChemSep to our model, pressure of condenser and column, heat loss, efficiency and also another parameter like ratio of Feed/Bottom.
2.6. Run the simulator

After all data is input and looks as green checklist then click the triangle green below the solve options in tab. Then the result before modification is following as Fig. 7:

From the picture we can see that ChemSep has possibility and ability to upgrade the requirement mass flow of the mass transfer. So, the condition operation has chance to maximalize the quality of product and maximize the efficiency of the equipment.
3. Result and Discussion

Refers to, Wankat. 2006. ChemSep can be optimization the separation also for azeotrope distillation. Such as Water and Ethanol can be separately as the requirement. By setting the condition operation, ChemSep can modify the mole fraction of the output to get the best operation as the practicant need [15].

Optimization of operating conditions is a method to determine the most optimum operating conditions in order to produce the desired product so that it has a high selling value and also has a relatively cheaper repair price. especially in the case of polymerization in the distillation column, deposits such as polymers greatly influence the operation of the column itself. The following table below announced the operation condition between normal and after optimization:

| Pressure (Torr) | Temperature (°C) | Mole Fraction Poly AA |
|----------------|------------------|-----------------------|
| 20,5           | 120              | 5.8448E−09            |
| 21             | 120              | 5.8551E−09            |
| 21,5           | 120              | 5.8651E−09            |
| 22             | 120              | 5.8747E−09            |
| 22,5           | 120              | 5.8840E−09            |
| 23             | 120              | 5.8930E−09            |
| 23,5           | 120              | 5.9017E−09            |
| 24             | 120              | 4.9630E−24            |
| 24,5           | 120              | 5.7902E−24            |
| 25             | 120              | 2.9631E−09            |

From the table 1. We can see that at pressure 24 torr is the best condition to get the lowest polymer composition. So it can be used for the next step to optimize the combination by using the pressure.

From the table 2. we can see the combination of condition operation has been moderately optimize and see that the poly acrylic acid is flowing to the product and has been in the different. Nowwithstanding on the actual plant, the polymer has to decrease as possible as can be. By using ChemSep, we can provide that 17 iterations is clearly get result of the composition of mole fraction needed. The result is different depend on the condition operation input.

| Trial | Pressure (torr) | Temperature (°C) | Mole Fraction 2-EHA | Poly AA |
|-------|----------------|------------------|---------------------|---------|
| Normal| 20             | 120              | 0.998144            | 5.8342E−09 |
| 1     | 23             | 120              | 0.998154            | 5.89E−09 |
| 2     | 24             | 120              | 0.998158            | 5.79E−24 |
| 3     | 24             | 121              | 0.998154            | 5.91E−09 |
| 4     | 24             | 124              | 0.998143            | 5.91E−09 |
| 5     | 24             | 125              | 0.998141            | 7.75E−21 |
| 6     | 25             | 120              | 0.998162            | 2.9631E−09 |
| 7     | 30             | 120              | 0.99818             | 2.9965E−09 |
4. Conclusion
The data improve of the amount poly acrylic content in the column distillation and also can be decrease more if there is continue investigation and more trial. Nevertheless, ChemSep can also simulate the poly acrylic acid for decreasing the content. The best condition operation after optimization is 24 torr and temperature 120°C with polymer content of 5, 79e – 24 mole fraction.

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