Simulation of Liquid Vapor Equilibrium in Batch Distillation Process from Cellulose (Bamboo)

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Abstract

Simulation of batch distillation binary systems using matlab programming language, which results in the appearance of the graph using a spreadsheet tool, less effective and efficient, so it is necessary for the visualization of object-oriented programming language, in addition to easy to be developed at a time when that will come, it has other benefits, in a device project software can use a variety of programming language that supports object-oriented programming, such as C#.Net and VB.Net. This research aims to display the batch distillation simulation of visual binary systems using Mat lab programming. Ethanol-water azeotropic binary system examples and Acetone-Butanol, Acetone-Ethanol, Butanol-Ethanol azeotropic binary system examples, simulation of batch distillation with rigorous method using a model Differential-Algebraic-Equations (DAEs), where liquid vapor equilibrium in batch distillation process from cellulose (Bamboo) with Antoine equation. Profile of liquida composition and vapor composition function dimensionless can be displayed directly from the desktop, to have the azeotropic binary system value profile activity coefficient is not equal to one, while the binary system azeotropic approaching one. Profile of liquida composition and vapor composition maximum from binary system azeotropic is 0.98, while for the binary system azeotropic approaching one. Economically using Mat lab language faster, time efficiency and better performance profile.

Keywords: Antoine, bamboo, binary systems, simulation

INTRODUCTION

At first batch distillation is used to separate the binary mixture is a mixture of HCl-H2O, H2SO4-H2O, NH3-H2O. The assumptions used are completely mixed liquida on still-pot, condensation using a total condenser and relative volatility (α) is considered constant, studied by Handogo and Wibawa (1997) and then written in the manual Separation Process Principles by Henley and Seader (1998). In the chemical industry, fermentation process is one way to get a chemical compound with the help of microorganisms helped, fermentation products enter the next stage of separation. At this stage it is important to produce a product with a certain purity, one of the common tools used in the separation process is a batch distillation column. Industrial separation processes in general separation of multicomponent and binary separation rare, therefore it is very important to review the multicomponent batch distillation. Design of multi-component batch distillation generally obtained by performing the simulation, in order to obtain the simulation results are close to the actual state of the accurate thermodynamic data needed (Prausnitz, 2001).

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In the separation process, thermodynamic data is the most dominant effect on the performance of the process is the equilibrium phase. One of the modern thermodynamic correlations in behavior percentage mix is not ideal UNIQUAC equation, the estimated equilibrium ternary and resource potential, economic, social and cultural infrastructure and institutional is yet to be optimal, 2) unpatched resource potential due to unexplored exploration, information and data, and, 3) no formulation model women fishermen empowerment based on local potential that can improve the welfare of fishermen community in Sidoarjo regency and able to contribute in regional development, especially in Sidoarjo regency. Quaternary systems can be done only by the experimental data of binary systems. Activity coefficient models with UNIQUAC equation was developed from a mixture of binary, and has advantages for application in multicomponent mixture system because it only requires binary parameters (does not require additional parameters). But the loss is not always successful models in predicting the multi-component equilibrium system shows a mixture which is not ideal especially for couples with a mix that has limited solubility such as butanol-water. To overcome this necessary equilibrium data measurement binary system accurately and the model estimates the parameters of the model so that the activity coefficient of these parameters can be used to estimate the vapor-liquid equilibrium multi-component system accurately (Widagdo and Warren, 1996).

Simulation of batch distillation binary system has been investigated using rigorous methods to DAEs models, where the completion of the model equations numerically using the Euler method using MatLab language version 6.1 (Attarakih et al., 2012). Results of the simulation system binary system acetone-butanol, acetone-ethanol, ethanol-butanol and then validated with a binary system of benzene-toluene.

Along with the development of information technology, the program may evolve over time using the programming methods applied lately that pemorgaman object-oriented, in addition to easy to be developed at a time when that will come, the software uses object-oriented programming methods this has other benefits, too in 1 software projects can use a variety of programming languages that support object oriented programming, such as C#.Net and VB.Net.

Simulation of batch distillation of binary systems using matlab programming language, which results in the appearance of the graph using a spreadsheet tool, less effective and efficient (Attarakih et al., 2012), so it is necessary for the visualization of object oriented programming language, in addition to easily be developed at a time when that will come, have another advantage is in the software projects can use a variety of programming language that supports object-oriented programming, such as C#.Net and VB.Net (Ni Ketut et al., 2013).

This research aims to display simulation profile liquida composition and vapor composition function dimensionless with Antoine equation in batch distillation process use Mat lab programming.

**METHODS**

Basic concepts of Object Oriented Programming concepts emphasize the following:

*Class*: the collection of data definitions and functions in a unit for a particular purpose. Class is the basis of modularity and structure in an object-oriented programming. A class should typically be recognizable by even a non-programmer domain associated with the existing problems, and the code is contained in a class should be (relatively) autonomous and independent nature (as the code is used if not using OOP). With modularity, the structure of a program will be associated with aspects of the problem to be solved through the program. This way will simplify the mapping of the problem to a program or vice versa (Aristarchus et al., 2011). *Object*: wrapping the data and functions together into a unit in a computer program, object is the basis of modularity and structure in an object oriented computer program. *Abstraction*: The ability of a program to bypass aspects of the information processed by it, namely the ability to focus on the core (Aristarchus et al., 2011). *Encapsulation*: Ensuring the user of an object can not change the state of an object in a way that is not feasible; just the method in which the object was given permission to access the situation.
Polymorphism: through sending messages. Does not depend on calling subroutines, object-oriented language can send messages; particular method associated with a message delivery depends on the specific object in which the beam is sent. For example, if a bird receive "fast motion", he would move his wings and fly. When a lion received the same message, he will move his legs and ran. Both answered a similar message, but in accordance with the ability of these animals. This is called polymorphism as a variable in the program tungal can hold different types of objects while running the program, and the text of the same program can call several different methods at different times in the same calling.

This is in contrast to functional languages achieve polymorphism through the use of first-class functions. By using the OOP in solving a problem we do not see how to solve a problem is objects but what can be done solving those problems. For example, suppose we have a department that has a manager, secretary, data and other administration officials. Suppose the manager wants to obtain data from the administrative manager of the bag does not have to take it immediately but can be ordered officers to take administrative bag. In that case, a manager does not have to know how to take the data, but the manager can get the data object through administrative officer. So in order to solve a problem with collaboration among existing objects because each object has its own job description.

In making the application is used batch distillation program makers and the language used to create the program: Visual Studio 2010 is a developer of software (Software Maker) issued by one of the largest computer software company in the world that is Microsoft. The advantage of this is that Visual Studio 2010 has been adopted. Net Framework 4.0 and the many languages that can be used to create such software, such as C#.Net, VB.Net, and so forth. Microsoft.NET Framework (Microsoft Dot Net Framework) or better known as the dot net is a software framework that runs primarily on Microsoft’s Windows operating system, this time. NET Framework generally have been integrated in the standard distribution of Windows (starting from Windows Server 2003 Windows versions and newer). The framework provides a large amount of computer programming libraries and supports several programming languages and good interoperability allowing these languages to serve one another in the development of the system.

At low pressure, the vapor phase so close to the ideal gas low pressure liquid vapor equilibrium becomes,

\[
y'_{i} = \frac{y_{i} \cdot P}{x_{i} \cdot P_{sat}^{i}}
\]  

Equation (1) is also known as the modified Raoult's equation. The constant of equilibrium between the vapor phase and liquid phase is defined as follows:

\[
K_{i} = \frac{y_{i}}{x_{i}} = \frac{y_{i} \cdot P_{sat}^{i}}{P}
\]  

Iteration procedure to find the temperature of which is to seek price bubble saturation temperature of pure component Tisat on P (Prausnitz et al., 2001).
\[ T_{i}^{\text{sat}} = \frac{B_i}{A_i - \log P_i} - C_i \]  

(3)

where A, B, C are Antoine constants for species \( i \), for all initial estimates.

\[ T = \sum_{i} x_i T_{i}^{\text{sat}} \]  

(4)

Price \( T \) as the initial price will be used to determine the saturated vapor pressure of a substance to be estimated with the equation \( T \) Antoine. Sedangkan prices were sought by the equation:

\[ T = \frac{B_j}{A_j - \log P_j^{\text{sat}}} - C_j \]  

(5)

Then look for the error between the new \( T \) with \( T \) the beginning with equation

\[ \left| \frac{T_{\text{new}} - T_{\text{beginning}}}{T_{\text{new}}} \right| \leq e \]  

(6)

Table 1. The feed composition of acetone Butanol

| Run | Acetone | Butanol |
|-----|---------|---------|
| 1   | 0,8     | 0,2     |
| 2   | 0,7     | 0,3     |
| 3   | 0,6     | 0,4     |
| 4   | 0,5     | 0,5     |
| 5   | 0,4     | 0,6     |
| 6   | 0,3     | 0,7     |
| 7   | 0,2     | 0,8     |

Source: Prausnitz, 2001
For other feed components such as: ethanol-water, acetone-ethanol, butanol-ethanol and benzene-toluene idem as Table 1.

Table 2. Antoine parameters acetone-butanol- ethanol-benzene-toluene

| Components       | A     | B     | C     |
|------------------|-------|-------|-------|
| Acetone          | 4.2184| 4.6493| 5.3365|
| Butanol          | 197.01| 1395.14| 1684.22|
| Ethanol          | 228.06| 182.739| 230.918|
| Benzene          | 3.98523| 1184.24| 217.572|
| Toluene          | 4.05043| 1237.62| 217.625|

To calculate the saturated vapor pressure Antoine equation is used data Antoine parameters such as Table 2. (Prausnitz, 2001), where the temperature (T) in units of K and saturated vapor pressure (PSAT) in units of Bar.

RESULT AND DISCUSSION

Figure 1 until Figure 3 are the profiles obtained using a spreadsheet tool, the simulation results of batch distillation binary system using Mathlab programming language. Temperature profile at the bottom shows results close to the temperature in the distillate, as a simple batch distillation process operates under total reflux conditions. Therefore, the temperature profile simulation results shown in Figure 1 is the number component-i temperature after normalization multiplied in the bottom component-i composition liquida. Figure 1 shows the temperature profile for the acetone-butanol Run 1 to Run-7 as a whole rose against dimensionless time. This is because the components are vaporized by the larger portion is a component of acetone, so it takes a greater temperature to evaporate the water component that has not evaporated.

![Temperature profile](image)

Figure 1. Women fishermen empowerment based on local potentials

From Figure 2 shows the composition profile in the bottom liquida for Run-1 shows the composition of the acetone decreased from the initial composition profile and butanol composition profile shows up on the initial composition. Because components while acetone is a volatile component of the butanol component is non-volatile components, at the time of batch distillation processes volatile components in a larger portion was evaporated and the remainder is non-volatile components.
Both components showed a constant composition profiles at dimensionless time showed a value of 2.5. This is due to the high boiling point butanol thus affecting the temperature of a mixture between the two components, thus both components of acetone and butanol components in large portions evaporate.

From Figure 3 shows the composition profile in the bottom liquida for Run-1, the total reflux condition to calculate the composition of benzene and toluene in the bottom composition of the initial temperature of 25 °C and composition determined benzene and toluene composition is determined, then calculated based on the bubble-point. At the time of total reflux composition of benzene and toluene in the bottom composition is not the same as the composition of benzene and toluene at the beginning. Composition profile shows benzene decreased from the starting composition and the composition of the toluene composition profile shows up from the beginning, because the composition of benzene is a volatile component of the component, while toluene is non-volatile components, at the time of batch distillation processes volatile component in a larger portion was evaporated and the remainder is non-volatile components. At the bottom of the composition profiles for acetone-butanol have shown a trend that is almost close to the composition profile at the bottom of benzene-toluene, so that the whole can meet the expected validation.
CONCLUSION

Temperature profile of the binary system as a whole was up against the dimensionless time, except at the beginning of the process shows the temperature profile decreases, due to the nature of the characteristics of the separated mixture. Liquida composition profile in the bottom for Run-1 to Run-7 shows the composition of non-volatile pure approach with dimensionless time of 3.5. Vapor composition profiles in the bottom close to the same as the composition profiles liquida at bottom, except at the beginning of the process of composition is evaporated more volatile.

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