Simulation of Activity Coefficient System Ternary in Acetone Buthanol Ethanol with Uniquac Equation

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ABSTRACT

Simulation of activity coefficients ternary 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 object-oriented programming. Ethanol buthanol ethanol non azeotropic ternary system, simulation of activity coefficients with rigorous method using a model Differential-Algebraic-Equations (DAEs), where the completion of the model using the language C#.Net, the basic concepts of object-oriented programming consists of classes, objects, abstraction, encapsulation, polymorphism. Antoine parameter data and activity coefficients derived from experimental data. Dimension less time and pressure are set constant, while the variable composition liquida. Profile of liquida composition and vapor composition function dimensionless can be displayed directly from the desktop, to have the non azeotropic ternary system value profile activity coefficient is not equal to one, while the ternary system non azeotropic approaching one. Profile of liquida composition and vapor composition maximum from ternary system non azeotropic is 0.98, while for the ternary system non aeotropic approaching one. Economically using C#.Net language faster, time efficiency and better performance profile.

Keywords: Activity Coefficients, C#.Net, Daes, Rigorous Method, Ternary Systems

1. 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 Rayleigh (1902) 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 (Sari, 2009). 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 (Widagdo & Seider, 1996).

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 mempersentasikan mix is not ideal UNIQUAC equation, the estimated

equilibrium ternary and 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 multi-component 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 (Renanto, 1997).

Simulation of activities coefficients equation ternary 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 (Sari, 2006). 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 objeck 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 (Sari et al., 2007), 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 Sari, et al., 2013)

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

2. Research Method

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 (Aristarchus et al., 2011). *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 (Aristarchus et al., 2011).

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 received "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 (Aristarchus et al., 2011).

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,

$$\gamma_i = \frac{y_i . P}{x_i . P_i^{sat}} \quad (1)$$

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:

$$K_i = \frac{y_i}{x_i} = \frac{\gamma_i . P_i^{sat}}{P} \quad (2)$$

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).

$$T_i^{sat} = \frac{B_i}{A_i - \log P} - C_i \quad (3)$$

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

$$T = \sum_i x_i T_i^{sat} \quad (4)$$

For i = 1, 2, 3.

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:

$$T = \frac{B_j}{A_j - \log P_1^{sat}} - C_j \quad (5)$$

Then look for the error between the new T with T the beginning with equation (6)

$$\left| \frac{(T_{new} - T_{beginning})}{T_{new}} \right| \leq e \quad (6)$$

Table 2. Antoine parameters acetone-butanol- ethanol-benzene-toluene
***Source: Prausnitz*. 2001**

γ_i activity coefficients obtained from:

$$\ln \gamma_i = \ln \gamma_i^C + \ln \gamma_i^R \quad (7)$$

$$\ln\gamma_i^C = \ln\frac{\varphi_i}{x_i} + \frac{z}{2} q_i \ln\frac{\theta_i}{\varphi_i} + \ell_i - \frac{\varphi_i}{x_i}\sum_{j=1}^{m} x_j \ell_j \quad (8)$$

$$\ln\gamma_i^R = q_i\left[1 - \ln\left(\sum_{j=1}^{m}\theta_j\tau_{ji}\right) - \sum_{j=1}^{m}\frac{\theta_j\tau_{ij}}{\sum_{k=1}^{m}\theta_k\tau_{kj}}\right] \quad (9)$$

$$\ell_i = \frac{z}{2}(r_i - q_i) - (r_i - 1) \quad (10)$$

where the coordination number z is set equal to 10.

$$\varphi_i = \frac{x_i r_i}{\sum_{j=1}^{m} x_j r_j} \quad (11)$$

$$\theta_i = \frac{q_i x_i}{\sum_{j=1}^{m} q_j x_j} \quad (12)$$

The parameters r, q is a constant component of the molecular structure based purely on molecular size and external surface area.
For each binary combination in multi-component mixtures, there are two parameters that can be adjusted r, q:

$$\tau_{ji} = \exp\frac{(u_{ji} - u_{ii})}{RT} \quad (13)$$

	Parameters Antoine		
Components	A	B	C
Acetone	4.2184	4.6493	5.3365
Butanol	197.01	1395.14	1648.22
Ethanol	228.06	182.739	230.918
Benzene	3.98523	1184.24	217.572
Toluene	4.05043	1327.62	217.625

$\tau_{jj} = \tau_{ii} = 1$

To calculate the saturated vapor pressure Antoine equation is used data Antoine parameters such as Table 1. (Prausnitz, 2001), where the temperature (T) in units of K and saturated vapor pressure (PSAT) in units of Bar.

3. Results 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.

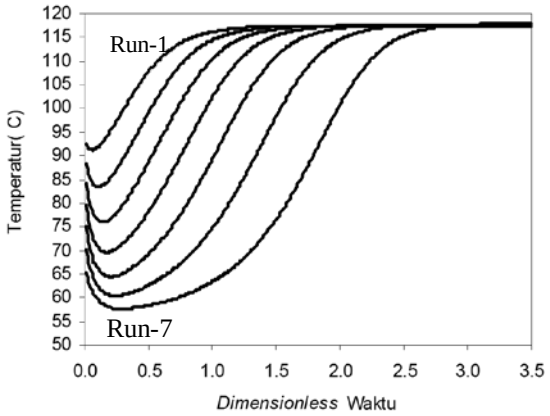

Figure 1. Temperature profile of Acetone Buthanol Ethanol Ternary System for Run-1 to Run-7.

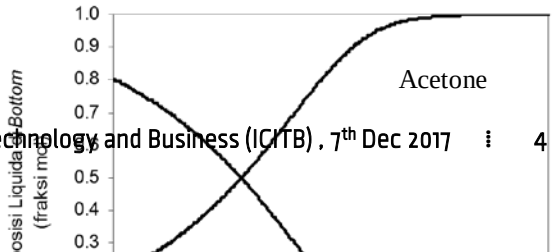

Figure 2. Composition Profile in the Bottom Liquida Acetone-Butanol

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.

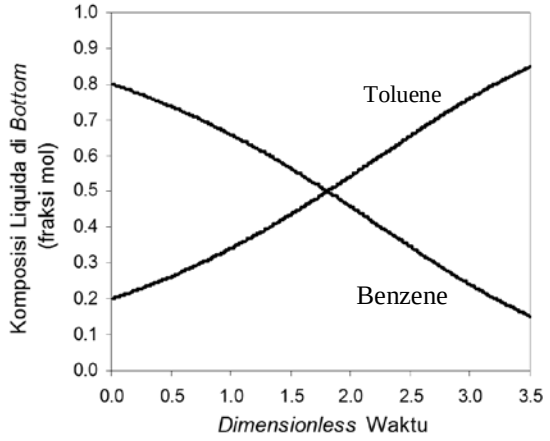

Figure 3. Composition Profile in the Bottom Liquida benzene-toluene.

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 ^{0}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.

4. Conclusion

Temperature profile 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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