Comparison of Activity Coefficient in ABE with MEP with UNIQUAC Equation

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Abstract: UNIQUAC equations in calculating the activity coefficient Acetone Butanol Ethanol (ABE) ternary system using the Mat-lab programming language, then verified with a homologous series of alcohol Methanol Ethanol Propanol (MEP) ternary system, to see if the mixture is an ideal or non-ideal solution. If the activity coefficient is close to one, then the solution is the ideal solution, whereas if the activity coefficient is more or less one, then the solution is a non-ideal solution so that in the separation of the solution, the activity coefficient should not be assumed to be the same as one, the activity coefficient should be calculated the actual value. The fixed variable consists of the temperature and Antoine parameter, the change variable consists of the liquid composition and dimensionless time, then obtained the activity coefficient profile function dimensionless time from the ABE and MEP ternary systems. With UNIQUAC equations obtained activity coefficients of the ABE ternary system more than once, while MEP ternary system shows the activity coefficient close to one, it can be concluded that the ABE ternary system is an a-zeotropic ternary system.

1 INTRODUCTION

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). Research by Rayleigh (1902) and later research by Henley and Seader (1998) book in the Principles of Separation Process. In the chemical industry, the solution separation process is an important process for collecting pure components, one of which uses thermodynamic theory of the coefficient of activity, to determine the ideal solution (Sari, 2018). In the separation process, thermodynamic data in the form of equilibrium data is very dominant in the solution separation process. One of the correlations of modern thermodynamics to the equilibrium phase that is not ideal is the UNIQUAC equation, the approximate balance and prediction data can only be obtained in the experimental data of binary systems. The coefficient model of ternary system activity with UNIQUAC equations is developed from a binary mixture, and has the advantage of application in a multi-component mixed system and requires no additional parameters. But the disadvantages of not always succeeding in predicting a mixed multi-component balance system are not ideal, especially mixtures that have limited solubility (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 Mat-Lab 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 program 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

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object oriented programming, such as C#.Net and VB.Net.

Simulation of batch distillation of binary systems using Mat-lab 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 (Sari, et al., 2013) .

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

2 MATERIAL AND METHODS

Basic concepts of Object Oriented Programming concepts emphasize the following (Aristarchus et al., 2011): **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. **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. **Encapsulation**: Ensuring the user of an object cannot 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 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 single 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,

$$\gamma_i = \frac{y_i \cdot P}{x_i \cdot P_i^{sat}} \tag{3}$$

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:

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

Iteration procedure to find the temperature of which is to seek price bubble saturation temperature of pure component Ti^{sat} on P (Prausnitz, et al., 2001: Sari and Dira 2017).

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

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

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

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, prices were sought by the equation:

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

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

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

γ_i activity coefficients obtained from:

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

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

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

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

where the coordination number z is set equal to 10.

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

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

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:

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

$$\tau_{jj} = \tau_{ii} = 1 \qquad (14)$$

Table 1: Antoine parameters Acetone-Butanol-Ethanol

Source: Prausnitz, 2001

	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

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 (P^{SAT}) in units of Bar.

Table 2: Feed composition of ABE

	Feed composition (mole fraction)		
No.	Acetone	Butanol	Ethanol
1	0,8	0,1	0,1
2	0,7	0,2	0,1
3	0,7	0,1	0,2
4	0,6	0,3	0,1
5	0,6	0,1	0,3
6	0,5	0,1	0,4
7	0,4	0,1	0,5

The composition of the bait is taken 7 runs, already represents the profile of the activity coefficient function ABE ternary system composition such as Table 2 (Sari and Dira, 2018).

Table 3: Feed composition of MEP

	Feed composition (fraction mole)		
Run	Methanol	Ethanol	Propanol
1	0,80	0,10	0,10
2	0,90	0,02	0,08
3	0,70	0,20	0,10
4	0,30	0,60	0,10
5	0,39	0,60	0,01
6	0,50	0,40	0,10

The composition of the bait is taken 6 runs, already represents the profile of the activity coefficient function ABE ternary system composition such as Table 3 (Sari and Dira, 2018).

3 RESULTS AND DISCUSSIONS

The temperature profile at the beginning of the process indicates the propyl decreases to dimensionless 0.25, as the adaptation process for the process runs continuously. Temperature increase up to dimensionless 2.5 for all composition feeds, for Run 2 and Run 4 shows the highest temperature achievement, because a large mixture of acetone and butanol around 0.9, for the composition feed (Run 4) that is volatile will indicate the highest temperature.

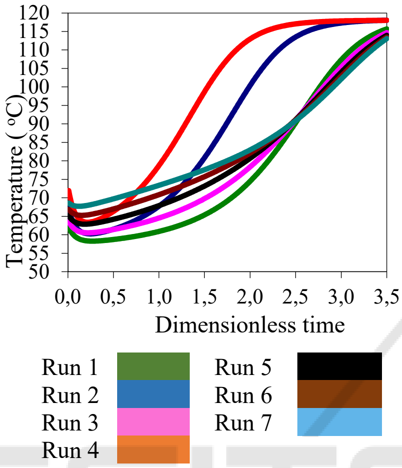

Figure 1: Profile temperature ABE versus dimensionless time

After dimensionless at a value of 3.5 all composition feeds show a flat profile, a temperature value with a range of 115 to 120 (°C), corresponding to the mixed temperature of the ABE ternary system, as shown in Figure 1.

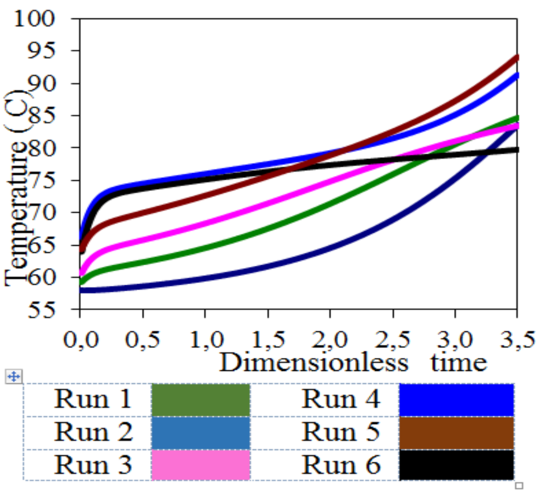

Figure 2: Profile temperature MEP versus dimensionless time

The temperature profile at the beginning of the process indicates the propyl decreases to dimensionless 0.25, as the adaptation process for the process runs continuously. Temperature increase up to dimensionless 3.5 for all composition feeds, for Run 6 shows the highest temperature achievement, because a large mixture of methanol and ethanol around 0.9, for the composition feed (Run 4) that is volatile will indicate the highest temperature. After dimensionless at a value of 3.5 all composition feeds show a flat profile, a temperature value with a range of 78 to 95 (°C), corresponding to the mixed temperature of the MEP ternary system, as shown in Figure 2.

At the beginning of the process until the activity coefficient shows a value of 1, Butanol and Ethanol show a decreased activity coefficient profile, Acetone shows a rising activity coefficient profile, all three approaching the ideal solution. At an activity coefficient value equal to 1.5 to 3.5, the activity coefficient profile of Butanol and Ethanol indicates an ideal solution, in which the process of separation of the mixture of activity coefficients can be assumed to be equal to 1. At an activity coefficient value equal to 1.5 to 3.5, the coefficient profile of Acetone, Butanol and Ethanol activity coefficient indicates no ideal solution, in which the process of separation of the mixture of activity coefficients should be calculated using UNIQUAC equations, as shown in Figure 3.

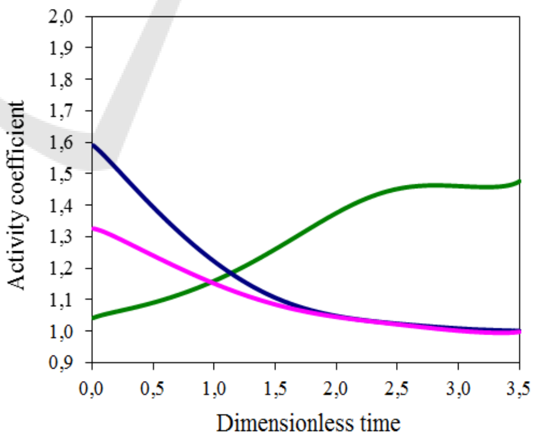

Figure 3: Profile activity coefficient of ABE versus dimensionless time

At the beginning of the process until the activity coefficient shows a value of 1, Methanol shows a decreased activity coefficient profile, Ethanol and Propanol show a rising activity coefficient profile, all three approaching the ideal solution. At an activity coefficient value equal to 1.5 to 3.5, the coefficient profile of Methanol, Ethanol and Propanol activity coefficient indicates no ideal solution, in which the process of separation of the mixture of activity coefficients should be calculated using UNIQUAC equations, as shown in Figure 4.

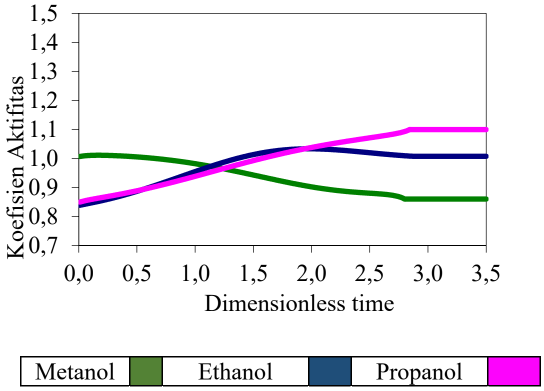

Figure 4: Profile activity coefficient of MEP versus dimensionless time

4 CONCLUSIONS

ABE temperature profile against dimensionless time shows the profile corresponding to the boiling point of each component, the temperature of range from 50 to 118 (^{O}C). ABE activity coefficient profile against dimensionless time (1.5 to 3.5) indicates a value not equal to 1, ABE is not an ideal solution, where in the process of separating ABE ternary system, the activity coefficient should be calculated using UNIQUAC equation. Verify the coefficient of ABE activities with the MEP activity coefficient against dimensionless time (1.5 to 3.5), indicating the dimensionless time value is not equal to 1, so that in the process of splitting the MEP ternary system, the activity coefficient must be calculated using UNIQUAC equations

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