



Simulation and Experimental System Terner Aseton-Butanol-Ethanol with Batch Distillation

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ABSTRACT

Result of Aseton-Butanol-Ethanol (ABE) ternary system simulation (ABE) in the form of temperature profile, liquid composition profile and vapour in bottom utilized as reference in ABE ternary system experiment, with komparasi result of ABE ternary system experiment and simulation will know how far deviation obtained.

For the dissociation of ABE ternary system done by research simulationly before done by research experimentally, so that in determination of research variable can more directional and expense of cheaper research. Simulation of ABE ternary system by batch distillation use rigorous method, model DAEs and Matlab language. Result of from ABE ternary system simulation later then comparison use Metanol-Ethanol-Propanol (MEP) ternary system which forming homolog deret. Usage of MEP ternary system in ABE ternary system comparison, because MEP ternary system mixture prediction form zeotropik mixture. Result of simulation in the form of temperature profile, liquid composition profile and vapor composition profile function of time dimensionless (ξ) either in bottom and also in distillate. Is afterwards done by ABE ternary system experiment with operating pressure 1 atmospher, ABE mixture volume 350 ml, ABE feed composition : 0.8, 0.1, 0.1 (mole fraction) and ξ : 0, 1, 2, 3.

Result of ABE ternary system simulation comparison with MEP ternary system come near result which same and show zeotropik mixture. Result of experiment and simulation in the form of temperature profile, liquid composition profile and vapor composition profile time dimensionless function either in bottom and also in distillate show result come near is samely. So that ABE ternary system simulation after comparison with MEP ternary system can wear by reference in ABE ternary system experiment

Keyword : time dimensionless, batch distillation, eksperiment, simulation, zeotropik

1. INTRODUCTION

In the chemical industry, the fermentation process is one way to get a chemical compound with the help of microorganisms, fermentation products enter the next stage of separation. At this stage it is very important to produce a product with a certain purity, one of the tools commonly used in the separation process is a batch distillation column. Separation process in the industry generally and the separation of multicomponent separation rarely binary, therefore it is important to review the multicomponent batch distillation. Design of multi-component batch distillation is generally obtained by performing simulations, in order to obtain simulation results are close to the actual state of the required thermodynamic data are accurate.

In the process of separation, thermodynamic data of the most dominant influence on the process performance is the equilibrium phase. One of the modern thermodynamic correlation in mempersentasikan behavior is not ideal mixture UNIQUAC equation, the approximate equilibrium ternary and quaternary systems can be done only based on experimental data of binary systems. Activity coefficient models with UNIQUAC equation was developed from a binary mixture, and has advantages

for applications in multi-component mixture system because it only requires a binary parameter (does not require additional parameters). But the loss model does not always succeed in predicting the equilibrium multi-component system that shows a mixture which is not ideal especially for mixtures that have a spouse with limited solubility such as butanol-water. To overcome these measurement data needed to accurately balance the binary system and model parameters estimation of activity coefficient models so that these parameters can be used to estimate the vapor-liquid equilibrium multi-component systems accurately.

From the simulation results obtained ternary system, to see the profile of the movement of the composition of liquid on the bottom then drawn in the form of residue curve maps. From the residue curve maps the ternary system can be known whether they form a ternary mixture zeotropik or azeotropic mixtures. Of the azeotropic mixture can be divided into homogeneous azeotropic mixtures and heterogeneous azeotropic mixtures. For homogeneous azeotropic mixture after separation of the results obtained form a single phase and azeotropnya point does not lie in Liquid-Liquid-Equilibrium (Mademoiselle), while for heterogeneous azeotropic mixture after separation of the results obtained form more than one phase and

azeotropnya point is at Mademoiselle. Then further developed for multi-component systems, namely in the form of residue curve maps of homogeneous and heterogeneous azeotropic mixture, the movement of the composition profile in the residue is formed liquida zeotropik or azeotropic mixtures. Ternary systems such as isopropanol-water-benzene to form a pseudo-homogeneous azeotropic mixtures have been studied by Pham and Doherty (1990). Ternary systems such as chloroform-benzene-acetone (Fidkowski et al. 1993), acetone-heptane-benzene (Henley and Seader, 1998), acetone-water-metyl ethyl ketone (Villiers et al. 2002) and isopropanol-methyl cyclohexane-toluene (Egbewatt and Fletcher 2003) to form a homogeneous azeotropic mixtures. Other ternary systems that form the heterogeneous azeotropic mixtures such as ethanol-water-benzene (Henley and Seader, 1998), ethanol-water-toluene (Henley and Seader, 1998). Other ternary systems such as nitrogen-argon-oxygen mixture without forming azeotropic or zeotropik, octane-2-ethoxy ethanol to form ethyl benzene azeotropic binary system, acetone-chloroform-methanol to form binary and ternary azeotropic system (Widagdo and Seider 1996). From the results of previous research, no one has made a map of residue curves for ternary mixtures ABE.

From the residue curve maps obtained and validated, the validation of the topological relations. To validate the topological relations using the equation that already exist in the literature (Henley and Seader, 1998). To determine whether the program listing the ternary system simulation is generally applicable, then validated based on data from the literature. Many ternary systems that already exist in the literature or journals that can be used for validation ABE ternary system, one of the ternary system used is a mixture that forms the ternary system zeotropik the MEP.

2. STRUCTURE OF WRITING

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

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

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:

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

Iteration procedure to find the temperature of which is to seek price bubble saturation temperature of pure component T_{isat} on P (Prausnitz et al., 2001).

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

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

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

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:

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

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

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

γ_i activity coefficients obtained from:

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

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

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

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

where the coordination number z is set equal to 10.

$$\phi_i = \frac{x_i \cdot r_i}{\sum_{j=1}^m x_j \cdot r_j} \dots\dots\dots (11)$$

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

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:

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

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

Model-Differential-Algebraic Equations (DAEs) for batch distillation of ternary system, assuming it does not form a two phase liquida by Doherty and Perkins (1978) as follows:

$$d\xi = \frac{-dx_i}{(x_i - y_i)} \dots\dots\dots (14)$$

$$\xi = \ln \left(\frac{W_o}{W} \right) \dots\dots\dots (15)$$

With a forward-finite-difference, Equation (15) becomes:

$$x_{i,j+1} = x_{i,j} + (y_{i,j} - x_{i,j}) \Delta\xi \dots\dots\dots (16)$$

Where the composition of the early liquida on the bottom (xi, j) and $\xi \Delta$ determined, while the composition of the vapor (yi, j) is calculated using Equation BUBL T (Prausnitz, 2001).

3. METHODOLOGY

To calculate the saturated vapor pressure Antoine equation is used, data Antoine parameters such as Table 3.2. (Prausnitz, 2001), where the temperature (T) in units of K and saturated vapor pressure (PSAT) in units of Bar. To calculate the activity coefficient (γ) using the UNIQUAC equation, where the price of UNIQUAC binary interaction parameters (uij), the volume of molecular data (r) and molecular surface area (q) Table 3.3, the assumption z = 10.

Table 3.1. ABE feed composition

Run	Komposisi Umpan (fraksi mol)		
	Aseton	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

Table 3.2. Antoine parameters ABE

Komponen	Parameter Antoine		
	A	B	C
Aseton	4.2184	4.6493	5.3365
Butanol	197.01	1395.14	1648.22
Ethanol	228.06	182.739	230.918

Source: Prausnitz, 2001

Table 3.3 Parameter UNIQUAC ABE system terner

Komponen	r	q
Aseton	2.5735	2.3359
Butanol	3.4542	3.0520
Ethanol	2.1054	1.9720

Source: Prausnitz, 2001

Dimana : Aseton (1), Butanol (2), Ethanol (3)

$$u_{11} = 0 \quad ; u_{12} = -198,659 \quad ; u_{13} = 98,75291$$

$$u_{21} = 453,669 \quad ; u_{22} = 0 \quad ; u_{23} = -32,707$$

$$u_{31} = 94,242 \quad ; u_{32} = 75,355 \quad ; u_{33} = 0$$

Validation of simulation results with the ternary system MEP

Table 3.4. MEP feed composition

Run	Komposisi Umpan (fraksi mol)		
	Metanol	Etanol	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

Sources: Henley and Seader, 1998

To calculate the saturated vapor pressure Antoine equation used

Table 3.5. Antoine parameters MEP

Komponen	Parameter Antoine		
	A	B	C
Metanol	5.20277	1580.08	239.500
Ethanol	228.06	182.739	230.918
Propanol	4.99991	1512.94	205.807

Sources: Prausnitz, 2001

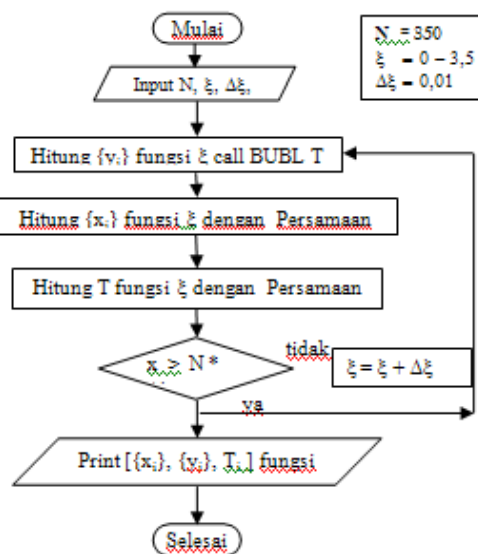


Figure 3.1. Batch distillation algorithm

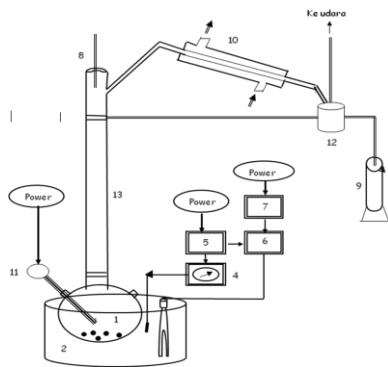


Figure 3.2. A set of batch distillation equipment

Caption:

1. Pot Still 8. Thermometer
2. Oil batch 9. glasses Measure
3. Heater 10. condenser
4. Thermocouple 11. thermocouple RTD
5. Controller 12. column separator
6. Contactor 13. packed column
7. regulators
7. Regulator

4. RESULTS AND DISCUSSIONS

Temperature profile at the bottom shows the results of the approach with temperatures in the distillate, because the simple batch distillation processes operate in conditions of total reflux. Therefore the temperature profile as Figure 4.1 simulation results is the sum of the *i*-component temperature after normalization multiplied in the bottom component of the composition of liquid-*i*. From Figure 4.1 shows the temperature profile for Run ABE-1 to Run-6 as a whole rose against the dimensionless time. This is because the components are evaporated with a larger portion is a component of ethanol, so it takes a larger temperature to evaporate the water component that has not evaporated.

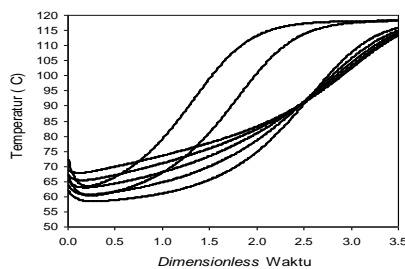


Figure 4.1 Profile of the temperature of the ternary system of ABE for Run-1 to Run-7

From Figure 4.2 is divided into 3 regions, for regions 1 shows the profile of water activity coefficient decreases and the activity coefficient of ethanol rises, so does not affect the temperature profile. Figure 4.2 shows that the larger the incoming feed water

composition on the influence of ethanol activity coefficient maximum at dimensionless time showed 1.75, after which profiles a constant decline in the end. The bigger the bait into the water composition showed a steeper slope of decline in temperature, because the composition of the bait into the water greatly affects the temperature of the mixture of ethanol-water-HCl, the greater the incoming feed water composition at the higher temperature of the mixture.

For region 2 the temperature profile rises for all the runs, the greater the ethanol composition in feed entry shows the temperature rise slope is more gentle. This is because the composition of the feed into ethanol greatly affects the temperature of the mixture of ethanol-water-HCl, the greater the ethanol composition in feed mixture into a temperature become smaller.

For region 3 the temperature profile rises and some constant, for the temperature profile rises mean the separation of a mixture of ethanol-water-HCl still exist that have not teruapkan ethanol, while for constant composition profile indicates that it is all teruapkan ethanol. The greater the composition of incoming feed water at the temperature of the mixture the greater and faster the temperature profile constant. For the dimensionless time of 3.5 the temperature profile has not been constant, so the dimensionless time required to obtain a larger constant temperature profile. If a simple batch distillation continued until the dimensionless time is very large, then the value will be the composition of each mixture is negative, this is not desired.

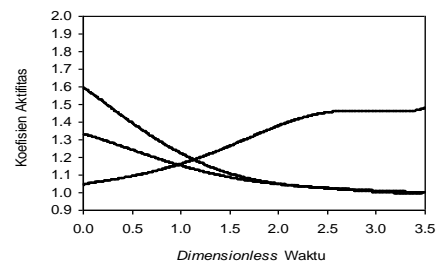


Figure 4.2 Profile of the activity coefficient of the ternary system of ABE

From Figure 4.3 shows the composition profile in the bottom liquid, the composition of ethanol shows the composition profile decreases from the initial composition and the composition of the water showed up from the initial composition profile.

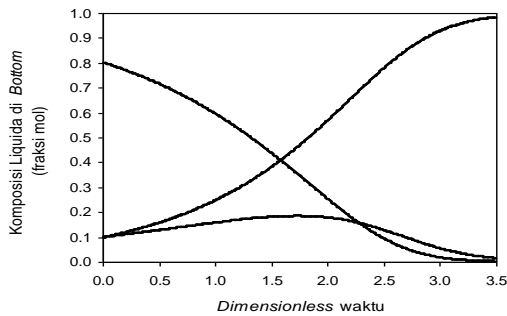


Figure 4.3. Liquida composition profiles in ternary systems ABE Bottom Run-1

Because ethanol is a component of volatile components while the water component is non-volatile components, as a simple batch distillation process of ethanol component in a larger portion is evaporated and the remaining components of the water. Component of pure water has not been approached with a dimensionless time of 3.5; one way to get more pure water component of the initial composition is to enlarge the composition of the feed water to enter.

Figure 4.4. shows the vapor composition profiles at total reflux for a bottom after the composition of ethanol continues to decline, while the composition of the water continues to rise. This disebabkan because volatile components were evaporated in a larger portion and the rest are non-volatile components, after a simple batch distillation process takes place then the non-volatile components are evaporated in a larger portion. Components of ethanol has not evaporate all at dimensionless time 3.5; one way to obtain the components of ethanol in the distillate with a smaller dimensionless time is to enlarge the composition of the feed water to enter. Vapor composition profiles at the bottom of small composition of ethanol on the feed entry, the greater the total composition of ethanol at reflux, this is due to a high temperature so that the mixture of non-volatile components evaporate more. Vapor composition profiles at total reflux for a bottom after the composition of ethanol continues to decline, while the composition of the water continues to rise. This disebabkan because volatile components were evaporated in a larger portion and the rest are non-volatile components, after a batch distillation process takes place then the non-volatile components are evaporated in a larger portion. Components of ethanol all teruapkan at dimensionless time shows the value of 2.25; Run-7 requires a smaller dimensionless time to obtain a more pure ethanol component of the initial

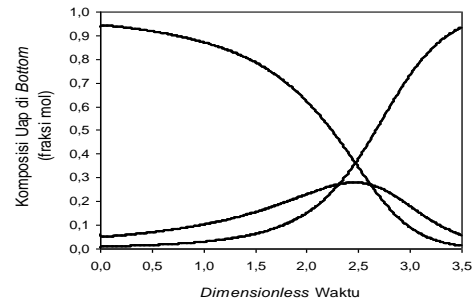


Figure 4.4. Vapor composition profiles in ternary systems ABE Bottom Run-1

Temperature profile at the bottom shows the results of the approach with temperatures in the distillate, because the simple batch distillation processes operate in conditions of total reflux. Therefore the temperature profile as Figure 4.5 simulation results is the sum of the i-component temperature after normalization multiplied in the bottom component of the composition of the liquida-i. From Figure 4.5 shows the temperature profile for Run MEP-1 to Run-6 as a whole rose against the dimensionless time. This is because the components

are evaporated with a larger portion is a component of ethanol, so it takes a larger temperature to evaporate the water component that has not evaporated.

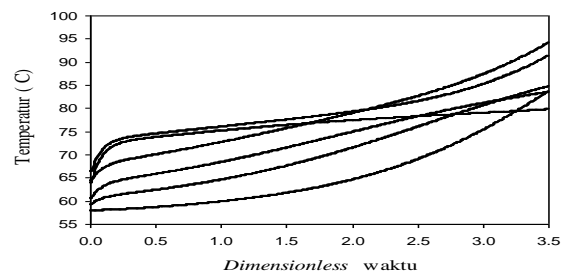


Figure 4.5 Profile of the temperature of the ternary system of MEP for Run-1 to Run-6

From Figure 4.6 is divided into 3 regions, for regions 1 shows the profile of water activity coefficient decreases and the activity coefficient of ethanol rises, so does not affect the temperature profile. Figure 4.6 shows that the larger the incoming feed water composition on the influence of ethanol activity coefficient maximum at dimensionless time showed 1.75, after which profiles a constant decline in the end. The bigger the bait into the water composition showed a steeper slope of decline in temperature, because the composition of incoming feed water at the temperature of the mixture greatly affects the MEP, the greater the incoming feed water composition at the higher temperature of the mixture.

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entry shows the temperature rise slope is more gentle. This is because the composition of the feed into ethanol greatly affects the temperature of the mixture of ethanol-water-HCl, the greater the ethanol composition in feed mixture into a temperature become smaller.

For region 3 the temperature profile rises and some constant, for the temperature profile rises mean the separation of a mixture of ethanol MEP still exist that have not teruapkan, while for constant composition profile indicates that it is all teruapkan ethanol. The greater the composition of incoming feed water at the temperature of the mixture the greater and faster the temperature profile constant. For the dimensionless time of 3.5 the temperature profile has not been constant, so the dimensionless time required to obtain a larger constant temperature profile. If a simple batch distillation continued until the dimensionless time is very large, then the value will be the composition of each mixture is negative, this is not desired.

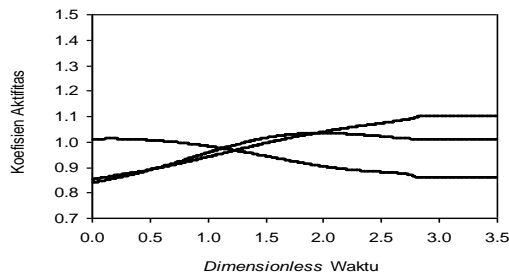


Figure 4.6. Ternary system activity coefficient profile MEP

From Figure 4.7 shows the composition profile in the bottom liquida, the composition of ethanol shows the composition profile decreases from the initial composition and the composition of the water showed up from the initial composition profile. Because ethanol is a component of volatile components while the water component is non-volatile components, as a simple batch distillation process of ethanol component in a larger portion is evaporated and the remaining components of the water. Component of pure water has not been approached with a dimensionless time of 3.5; one way to get more pure water component of the initial composition is to enlarge the composition of the feed water to enter.

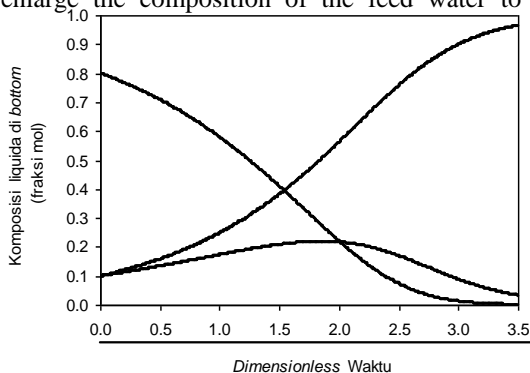


Figure 4.7. Composition profiles in the bottom liquida MEP ternary system Run-1

Figure 4.8. shows the vapor composition profiles at total reflux for a bottom after the composition of ethanol continues to decline, while the composition of the water continues to rise. This disebabkan because volatile components were evaporated in a larger portion and the rest are non-volatile components, after a simple batch distillation process takes place then the non-volatile components are evaporated in a larger portion. Ethanol components have not evaporate all at dimensionless time 3.5; one way to obtain the components of ethanol in the distillate with a smaller dimensionless time is to enlarge the composition of the feed water to enter. Vapor composition profiles at the bottom of small composition of ethanol on the feed entry, the greater the total composition of ethanol at reflux, this is due to a high temperature so that the mixture of non-volatile components evaporate more. Vapor composition profiles at total reflux for a bottom after the composition of ethanol continues to decline, while the composition of the water continues to rise. This disebabkan because volatile components were evaporated in a larger portion and the rest are non-volatile components, after a batch distillation process takes place then the non-volatile components are evaporated in a larger portion. Components of ethanol all teruapkan at dimensionless time shows the value of 2.25; Run-7 requires a smaller dimensionless time to obtain a more pure ethanol component of ethanol component of the initial

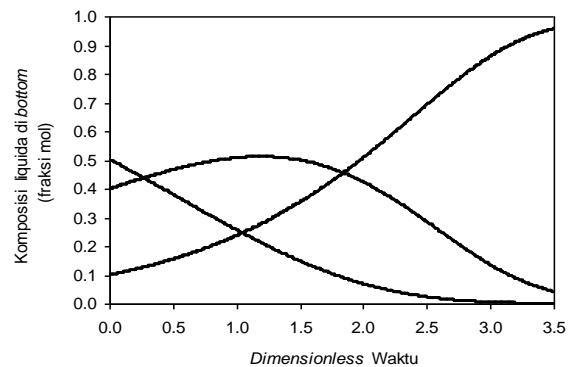


Figure 4.8. Vapor composition profiles in ternary systems bottom MEP Run-1 bl

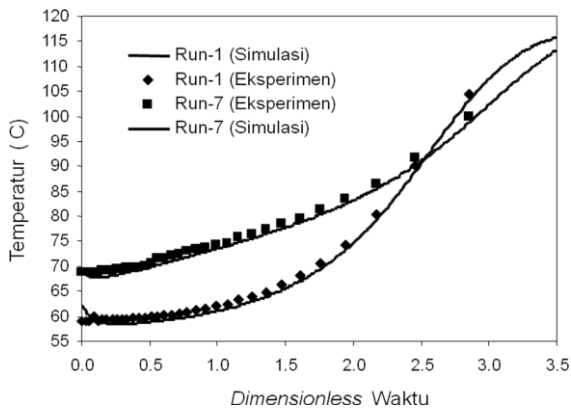


Figure 4.9 Profile of the temperature of the ternary system of ABE for Run-1, Run-7 simulation results and experimental

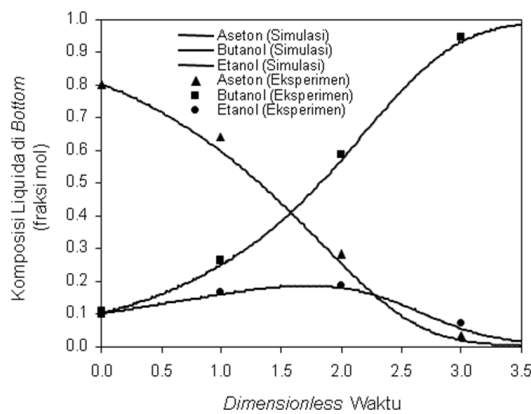


Figure 4.10. Liquida composition profiles in ternary systems bottom ABE-1 Run the simulation and experimental results

5. CONCLUSION

1. Ethanol-Water temperature profile-HCl as a whole rose 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 mixture.
2. Liquida composition profiles of ethanol in the bottom seteleh process shows the composition of a minimum of ethanol, after the process is complete profile constant composition
3. Ethanol vapor composition profiles in the bottom seteleh process showed a maximum ethanol composition, once the process is complete profile constant composition.
4. Residue curve map at bottom shows azeotropic mixture, between the simulation and validation results showed that close to the same profile

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