



# SOLVING THE DYNAMIC MODELS OF REACTIVE PACKED DISTILLATION PROCESS USING DIFFERENCE FORMULA APPROACHES

Abdulwahab GIWA

Department of Chemical Engineering, School of Engineering and Engineering Technology, Federal University of Technology, Gidan Kwano, Minna, Nigeria  
E-Mail: [a.giwa@futminna.edu.ng](mailto:a.giwa@futminna.edu.ng)

## ABSTRACT

One of the complex processes encountered in process industries is reactive distillation because it involves the integration of both reaction and separation in a single unit. The process becomes more complex if the column used is a packed type because, in that case, its dynamic models are combinations of both ordinary and partial differential equations. Obtaining the appropriate method that can reliably give the solutions of these complex dynamic models is one of the challenges facing Process Engineers. It has been discovered that difference formula approaches can be applied to convert the partial differential models of the process to ordinary differential model types so that the overall resulting ordinary differential dynamic models of the process can be solved with the aid of *ode* command of MATLAB. Therefore, this work has been carried out to demonstrate how backward, forward and central difference formula approaches involving two data points are applied in solving the dynamic models developed for the reactive packed distillation column used for the production of ethyl acetate. The results obtained from the solutions of the dynamic models using the three different difference formula approaches were compared to the measured ones to determine the reliability of each of the approaches in solving the dynamic models of the reactive packed distillation process and backward difference formula approach was discovered to be the best because the liquid ethyl acetate mole fraction and the top segment temperature it gave were found to compare very well with the measured values.

**Keywords:** dynamic model, difference formula, MATLAB, reactive distillation, ethyl acetate.

## 1. INTRODUCTION

Reactive distillation is a process that combines both separation and chemical reaction in a single unit. It is especially very attractive whenever conversion is limited by reaction equilibrium (Balasubramhanya and Doyle III, 2000; Giwa, 2012) because it combines the benefits of equilibrium reaction with distillation to enhance conversion provided that the product of interest has the highest or the lowest boiling point (Taylor and Krishna, 2000; Giwa, 2012). It has a lot of advantages which include reduced investment and operating costs due to increased yield of a reversible reaction by separating the product of interest from the reaction mixture (Pérez-Correa *et al.*, 2008; Giwa, 2012), high conversion, improved selectivity, low energy consumption, scope for difficult separations and avoidance of azeotropes (Jana and Adari, 2009; Giwa, 2012). Despite all these advantages, the solutions of the models of reactive distillation process are still challenges to Process Engineers especially when the column used is a packed type because, then, the models of the column are most likely to contain partial differential equations. As such, one of the methods discovered for handling these types of models is difference formula approach because they can be used to convert the partial differential equations into ordinary ones.

The formulation of the difference formulas involving two data points can be seen to be the outcome of considering the Taylor series expansion of a function of one variable  $f(x)$  as (Fausett, 2008):

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \dots \quad (1)$$

Neglecting the terms with orders from two,

$$f(x+h) = f(x) + hf'(x) \quad (2)$$

Therefore,

$$f(x+h) - f(x) = hf'(x) \quad (3)$$

$$hf'(x) = f(x+h) - f(x) \quad (4)$$

$$f'(x) = \frac{f(x+h) - f(x)}{h} \quad (5)$$

For forward difference, making  $h = x_{i+1} - x_i$ , for  $f(x) = f(x_i)$ , from Equation (5),

$$f'(x_i) = \frac{f(x_i + x_{i+1} - x_i) - f(x_i)}{x_{i+1} - x_i} \quad (6)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \quad (7)$$

For backward difference, making  $h = x_i - x_{i-1}$ , for  $f(x) = f(x_i)$ , from Equation (5),



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$$f'(x_i) = \frac{f(x_i + x_{i-1} - x_i) - f(x_i)}{x_{i-1} - x_i} \quad (8)$$

$$f'(x_i) = \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i} \quad (9)$$

For central difference, which is the average of the forward and the backward approximations, making  $h = +h$  in Equation (1),

$$f(x+h) - f(x-h) = f(x) - f(x) + hf'(x) - (-hf'(x)) + \frac{h^2}{2!} f''(x) - \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) - \left( -\frac{h^3}{3!} f'''(x) \right) + \dots \quad (12)$$

$$f(x+h) - f(x-h) = hf'(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^3}{3!} f'''(x) + \dots \quad (13)$$

$$f(x+h) - f(x-h) = 2hf'(x) + 2\frac{h^2}{2!} f''(x) + 2\frac{h^3}{3!} f'''(x) + \dots \quad (14)$$

Ignoring any term having order greater than or equal to 2,

$$f(x+h) - f(x-h) = 2hf'(x) \quad (15)$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) \quad (15)$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \quad (16)$$

For  $f(x) = f(x_i)$ , Equation (16) becomes,

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \quad (17)$$

Therefore, in this work, it is desired to apply the three different difference approaches, discussed above, involving two data points to the solutions of the models developed for the reactive packed distillation process for the production of ethyl acetate via esterification reaction between acetic acid and ethanol.

## 2. PROCEDURES

Considering the dynamic models of the reactive packed distillation column given in the work of Giwa and Karacan (2012), the three difference formula approaches were applied as outlined in the following subsections.

### 2.1. Backward difference formula approach

For  $j=1$ , that is, the condenser section of the column,

$$\frac{dx_j}{dt} = \frac{V_{j+1}y_{j+1} - (L_d + L_R)x_j}{M_j} \quad (18)$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \dots \quad (10)$$

Further making  $h = -h$  in Equation (1),

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \dots \quad (11)$$

Subtracting Equation (11) from (10),

For  $j = 2 : nfa - 1$ , that is, the rectifying section of the column, for liquid phase,

$$\frac{dx}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_j - x_{j-1}}{\Delta z} \right) - k_y a A_c (y_j^* - y_j) \right) \quad (19)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (20)$$

For  $j = nfa$ , that is, the acetic acid feed section,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} + V_{j+1}y_{j+1} + F_a x_{fa} - L_j x_j - V_j y_j}{M_j} \quad (21)$$

For  $j = nfa + 1 : nfe - 1$ , that is, the reaction section, for liquid phase,

$$\frac{dx_j}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_j - x_{j-1}}{\Delta z} \right) - k_y a A_c (y_j^* - y_j) + r_j' W_j \right) \quad (22)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (23)$$

For  $j = nfe$ , that is, the ethanol feed section,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} + V_{j+1}y_{j+1} + F_e x_{fe} - L_j x_j - V_j y_j}{M_j} \quad (24)$$

For  $j = nfe + 1 : n - 1$ , that is, the stripping section, for liquid phase,



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$$\frac{dx_j}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_j - x_{j-1}}{\Delta z} \right) - k_y a A_c (y_j^* - y_j) \right) \quad (25)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (26)$$

For  $j = n$ , that is, the reboiler section of the column,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} - L_jx_j - V_jy_j}{M_j} \quad (27)$$

## 2.2. Forward difference formula approach

For  $j=1$ , that is, the condenser section of the column,

$$\frac{dx_j}{dt} = \frac{V_{j+1}y_{j+1} - (L_d + L_R)x_j}{M_j} \quad (28)$$

For  $j=2:nfa-1$ , that is, the rectifying section of the column, for liquid phase,

For liquid phase,

$$\frac{dx}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_{j+1} - x_j}{\Delta z} \right) - k_y a A_c (y_j^* - y_j) \right) \quad (29)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (30)$$

For  $j = nfa$ , that is, the acetic acid feed section,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} + V_{j+1}y_{j+1} + F_a x_{fa} - L_jx_j - V_jy_j}{M_j} \quad (31)$$

For  $j = nfa + 1 : nfe - 1$ , that is, the reaction section, for liquid phase,

For liquid phase,

$$\frac{dx_j}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_{j+1} - x_j}{\Delta z} \right) - k_y a A_c (y_j^* - y_j) + r_j W_j \right) \quad (32)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (33)$$

For  $j = nfe$ , that is, the ethanol feed section,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} + V_{j+1}y_{j+1} + F_e x_{fe} - L_jx_j - V_jy_j}{M_j} \quad (34)$$

For  $j = nfe + 1 : n - 1$ , that is, the stripping section, for liquid phase,

For liquid phase,

$$\frac{dx_j}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_{j+1} - x_j}{\Delta z} \right) - k_y a A_c (y_j^* - y_j) \right) \quad (35)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (36)$$

For  $j = n$ , that is, the reboiler section of the column,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} - L_jx_j - V_jy_j}{M_j} \quad (37)$$

## 2.3. Central difference formula approach

For  $j=1$ , that is, the condenser section of the column,

$$\frac{dx_j}{dt} = \frac{V_{j+1}y_{j+1} - (L_d + L_R)x_j}{M_j} \quad (38)$$

For  $j=2:nfa-1$ , that is, the rectifying section of the column, for liquid phase,

For liquid phase,

$$\frac{dx}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_{j+1} - x_{j-1}}{2\Delta z} \right) - k_y a A_c (y_j^* - y_j) \right) \quad (39)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (40)$$

For  $j = nfa$ , that is, the acetic acid feed section,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} + V_{j+1}y_{j+1} + F_a x_{fa} - L_jx_j - V_jy_j}{M_j} \quad (41)$$



For  $j = nfa + 1 : nfe - 1$ , that is, the reaction section, for liquid phase,

For liquid phase,

$$\frac{dx_j}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_{j+1} - x_{j-1}}{2\Delta z} \right) - k_y a A_c (y_j^* - y_j) + r_j W_j \right) \quad (42)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (43)$$

For  $j = nfe$ , that is, the ethanol feed section,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} + V_{j+1}y_{j+1} + F_e x_{fe} - L_j x_j - V_j y_j}{M_j} \quad (44)$$

For  $j = nfe + 1 : n - 1$ , that is, the stripping section, for liquid phase,

For liquid phase,

$$\frac{dx_j}{dt} = \frac{1}{M_j} \left( L_j \left( \frac{x_{j+1} - x_{j-1}}{2\Delta z} \right) - k_y a A_c (y_j^* - y_j) \right) \quad (45)$$

For vapor phase,

$$\frac{dy_j}{dz} = \frac{k_y a A_c}{V_j} (y_j^* - y_j) \quad (46)$$

For  $j = n$ , that is, the reboiler section of the column,

$$\frac{dx_j}{dt} = \frac{L_{j-1}x_{j-1} - L_j x_j - V_j y_j}{M_j} \quad (47)$$

In addition, the equilibrium relationships employed in this work are as given below.

For each segment of the column, for  $i = 1 : m$ , (where  $m$  is the number of components), throughout the entire column,

$$y_i = K_i x_i \quad (48)$$

$$\sum_{i=1}^m y_i = 1 \quad (49)$$

$$\sum_{i=1}^m x_i = 1 \quad (50)$$

In addition, the Antoine expression was used to estimate the equilibrium temperature of the system. Given in Equation (51) below is the form of the expression obtained from Sinnott (2005);

$$\ln(p) = A - \frac{B}{T + C} \quad (51)$$

After the conversions of the models using the difference formula approaches, they were solved with the aid of MATLAB R2013a (Mathworks, 2013) using the data given in Table-1.

**Table-1.** Data used for the solution of the models.

Parameter	Value
Number of components	4
Number of column segment	19
Acetic acid feed segment number	7
Ethanol feed segment number	13
Operating pressure (mmHg)	760
Reflux ratio	2.6103
Acetic acid feed volumetric flow rate (mL/min)	20
Ethanol feed volumetric flow rate (mL/min)	10
Reboiler duty (Watt)	107
Column height (m)	1.5
Column diameter (m)	0.05
Catalyst surface area (m <sup>2</sup> /kg)	53000
Catalyst density (kg/m <sup>3</sup> )	770

Furthermore, after the solutions of the developed models of the reactive packed distillation process, a prototype plant developed with the aid of Aspen Plus was run using the same data given in Table-1 so as to be able to compare the simulation results with the measured ones. Owing to the fact that the desired product (ethyl acetate) was obtained from the top segment of the column, the top segment temperature and the mole fraction of the ethyl acetate obtained from the top segment of the column were used as the basis of the comparison.

### 3. RESULTS AND DISCUSSIONS

#### 3.1. Backward difference formula approach findings

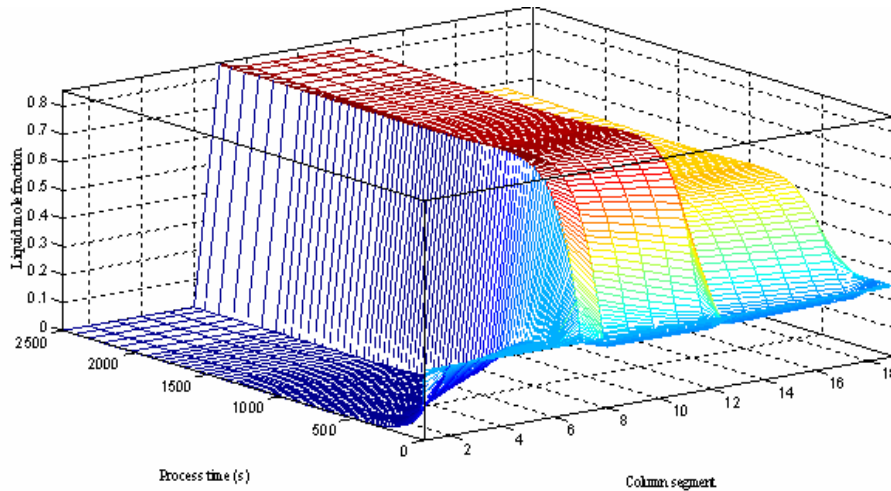
The results obtained from the solutions of the models developed for the reactive packed distillation process using the backward difference formula approach are as shown in Figures 1-4.

In Figure-1, the variation of the liquid mole fraction of acetic acid (a process reactant) obtained from the solution of the models of the process against the column segment and the process time is shown. As can be

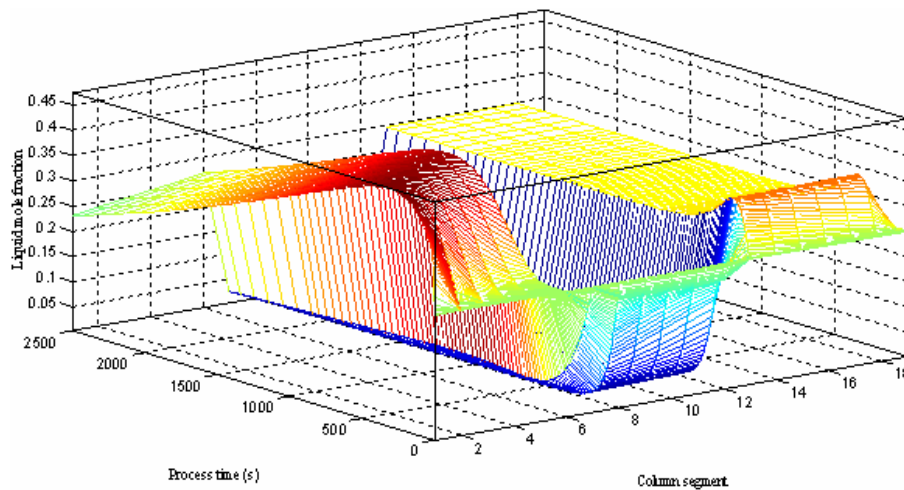


seen from the Figure, at the initial time of the process, considering the mole fractions, it was discovered that there were some acetic acid present along the entire column, from the top to the bottom. However, later on, at the process time of about 300 s, the acetic acid present at the

top segment of the column was found to be approximately zero while its (acetic acid's) maximum mole fraction was found to occur at the middle section of the column. This situation was found to remain almost like this till the end of the process time considered.



**Figure-1.** Acetic acid mole fraction in the reactive packed distillation column solved using backward difference approach.



**Figure-2.** Ethanol mole fraction in the reactive packed distillation column solved using backward difference approach.

The results shown in Figure-2 reveal the variation of liquid ethanol mole fraction with time and column segment, as obtained from the simulations of the developed models. As can be seen from the Figure, the mole fraction of ethanol (also, another reactant) was found to have its minimum at the middle (reaction section) of the column, especially after about 300 s of the simulation time, but at around the same time, it had its maximum mole fraction at the top segment of the column.

Considering the results given by Figures 1 and 2, it was seen that, while acetic acid had its maximum mole fraction at the middle section of the column, ethanol was found to have its minimum mole fraction at that segment.

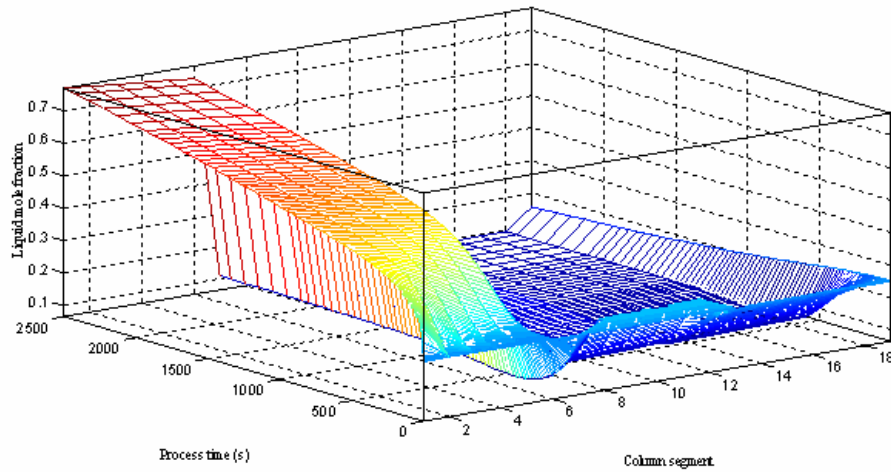
This was seen to mean that the unreacted ethanol, being more volatile than acetic acid, was able to move to the top segment of the column whereas the unreacted acetic acid, the less volatile reactant, was concentrating at the middle and at the bottom sections of the column.

The variation in liquid mole fraction of ethyl acetate (the desired product of the process) with time and column segment is as shown in Figure-3. From the Figure, it was observed that, at the top section of the column, the liquid mole fraction of ethyl acetate was increasing as the process simulation was proceeding. At the middle section of the column, the mole fraction of liquid ethyl acetate was found to be very minimal. This was found to mean that as

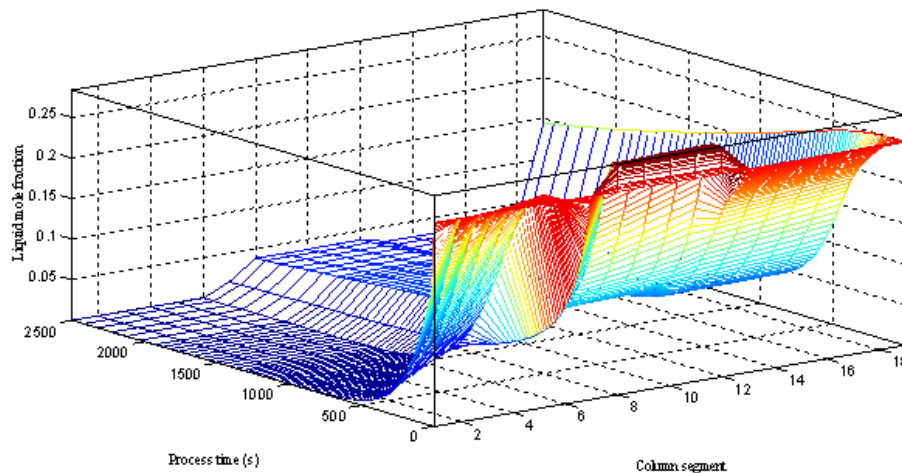


the desired product (ethyl acetate) was being produced in the reaction (middle) section of the column, being the

lightest of the components in the process, it was moving to the top segments of the column.



**Figure-3.** Ethyl acetate mole fraction in the reactive packed distillation column solved using backward difference approach.



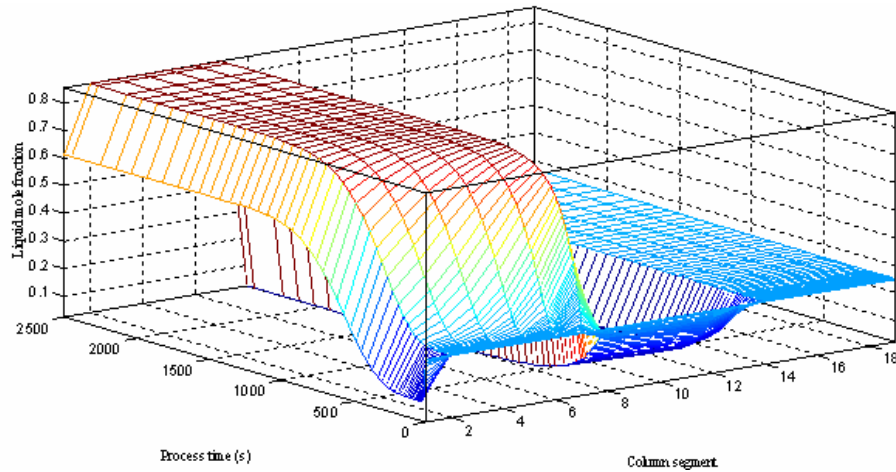
**Figure-4.** Water mole fraction in the reactive packed distillation column solved using backward difference approach.

The results shown in Figure-4 are for the variation of liquid mole fraction of water against process time and column segment. As can be seen from the figure, the mole fraction of water present in the column segments at the initial process time was found to be high, but it later decreased, even to the extent of decreasing to zero at the top segment of the column as the process time increased. At the end of the process simulation time, the segment of

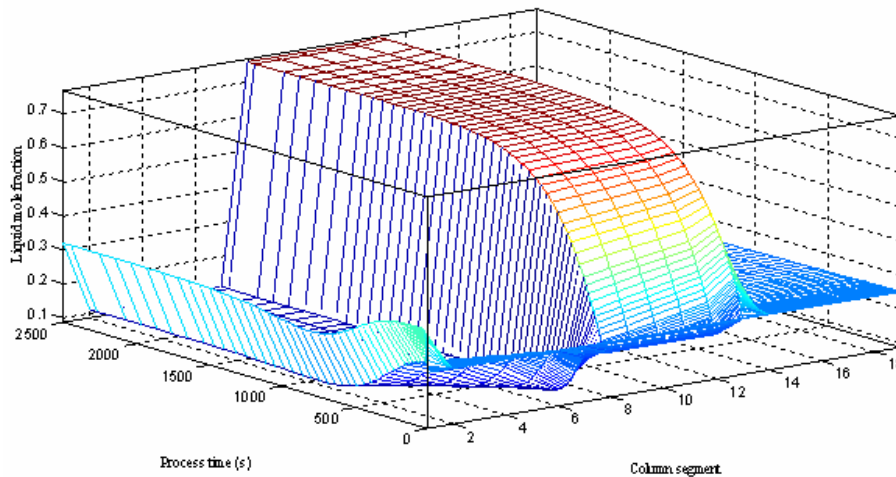
the column that had the highest liquid water mole fraction was found to be the bottom (reboiler) segment.

### 3.2. Forward difference formula approach findings

Shown in Figures 5-8 are the results obtained from the solutions of the developed models using forward difference formula approach.



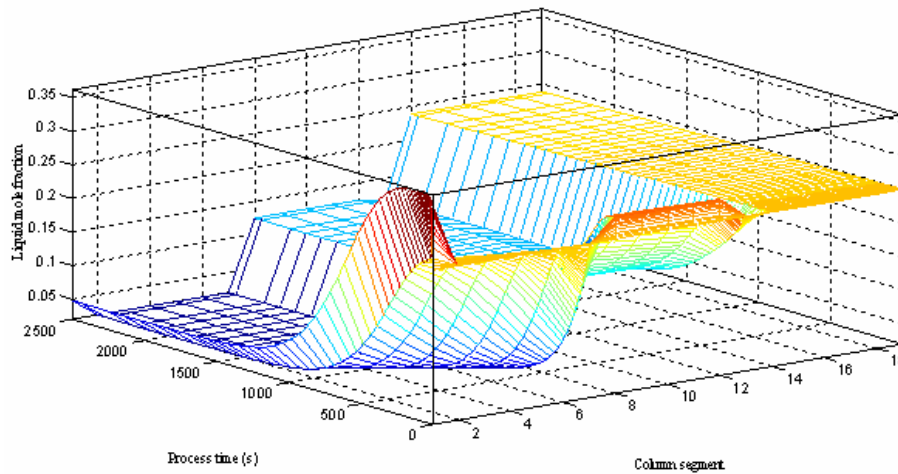
**Figure-5.** Acetic acid mole fraction in the reactive packed distillation column solved using forward difference approach.



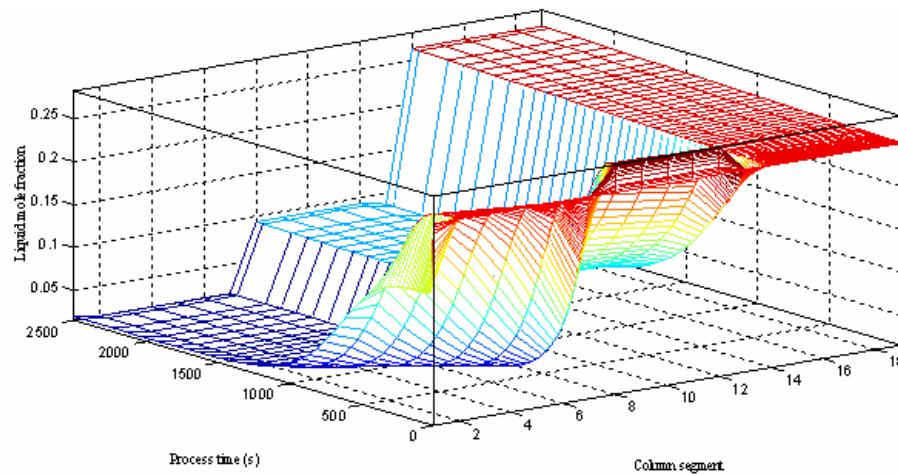
**Figure-6.** Ethanol mole fraction in the reactive packed distillation column solved using forward difference approach.

As can be seen in Figure-5 that shows the liquid mole fraction of acetic acid against process time and column segment obtained from the simulations of the process models using forward difference formula approach, it was observed that, in most of the process time, especially after about 500 s of the process time, the maximum mole fraction of acetic acid was found to be obtained at the top section of the column. Also, the minimum mole fraction of this component (acetic acid) obtained from the simulations carried out with the aid of forward difference formula approach was observed to be at the reaction section of the column while its mole

fraction at the bottom section was approximately constant in most of the simulation periods considered. Actually, the low mole fraction of acetic acid observed at the middle (reaction) section of the column was found to be favorable because that was pointing to the fact that there was no accumulation of acetic acid in that section. However, its high mole fraction found at the top section of the column made the observation obtained before to be doubtful because it could be that instead of acetic acid staying at the reaction section to participate in the production of ethyl acetate, it was evaporating to the top section of the column, unconverted.



**Figure-7.** Ethyl acetate mole fraction in the reactive packed distillation column solved using forward difference approach.



**Figure-8.** Water mole fraction in the reactive packed distillation column solved using forward difference approach.

Looking at the graph showing the variation of liquid mole fraction of ethanol with time along the segments of the column given in Figure-6, it was discovered that the highest ethanol mole fraction was found in the middle (reaction) section of the column. It should be remembered that it was at that section that the mole fraction of acetic acid (the other reactant) was the lowest. This has just shown that, according to the solution of this model by the forward difference formula approach, in the absence of acetic acid, since acetic acid was evaporating to the top section of the column instead of remaining in the reaction section for the reaction to take place, ethanol was being accumulated there (at the reaction section).

Now, considering the liquid mole fraction of the desired product (ethyl acetate) given in Figure-7 as a function of process time and column segment, it was

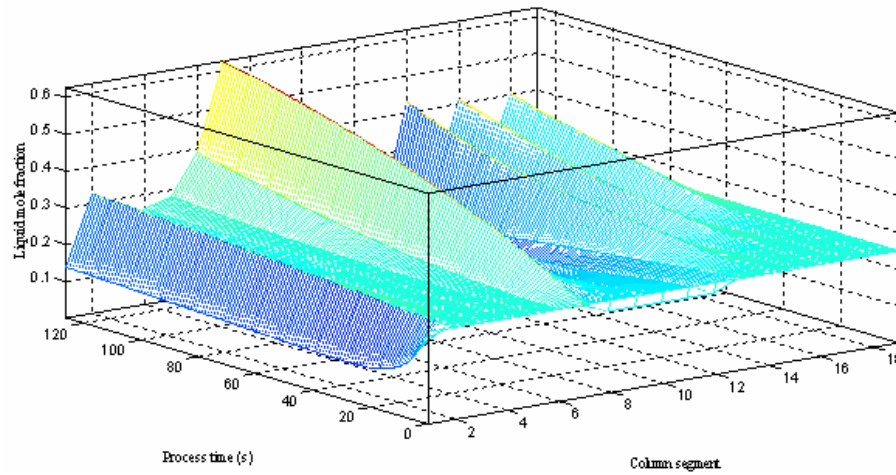
observed that the mole fraction (of ethyl acetate) present at the top segment of the column from where the product, being the lightest of the components involved in the process, was expected to be collected was very small.

From Figure-8 showing how the liquid water mole fraction obtained varied with process time and column segment, it was discovered that the highest mole fraction of the water produced by the process, as given by the simulations carried out, was present at the bottom section of the column while its lowest mole fraction was found to be at the column top section.

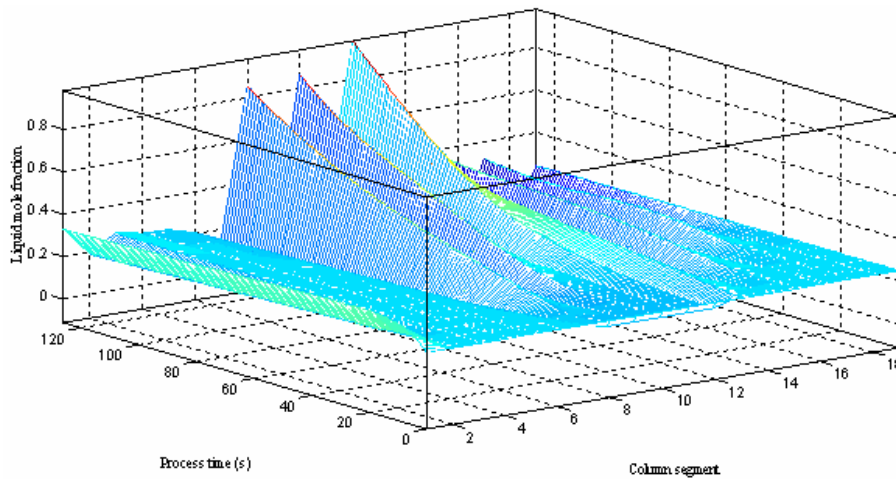
### 3.3. Central difference formula approach findings

Figures 9-12 show the liquid mole fraction of the components obtained from the solution of the models of the reactive packed distillation process using central difference formula approach.

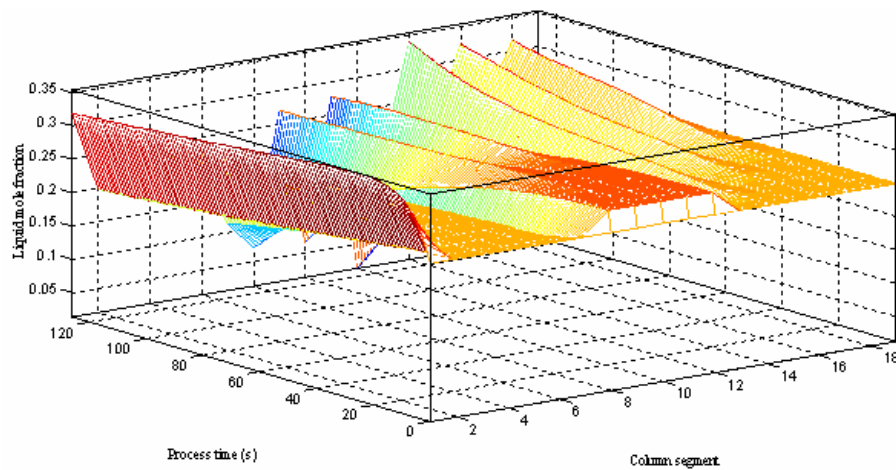




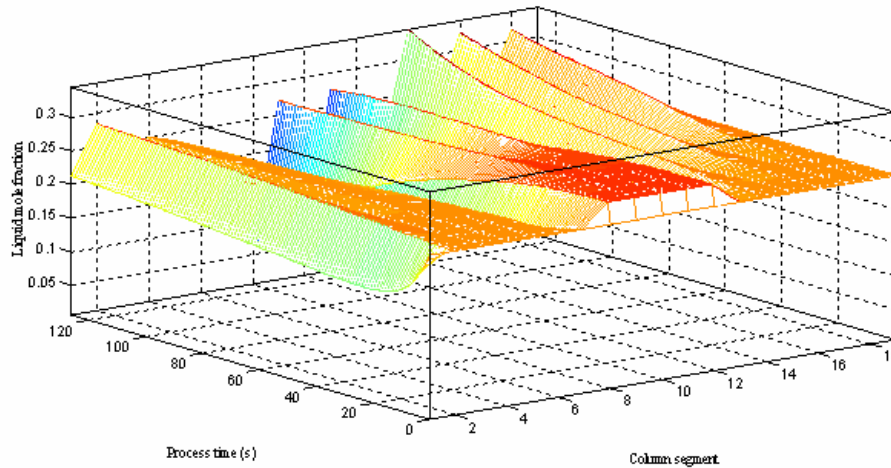
**Figure-9.** Acetic acid mole fraction in the reactive packed distillation column solved using central difference approach.



**Figure-10.** Ethanol mole fraction in the reactive packed distillation column solved using central difference approach.



**Figure-11.** Ethyl acetate mole fraction in the reactive packed distillation column solved using central difference approach.



**Figure-12.** Water mole fraction in the reactive packed distillation column solved using central difference approach.

According to the results shown in Figures 9-12, it was discovered that the natures of the mole fraction profiles of all the components involved in the process were similar and zigzag in nature. Based on the Figures, it could not be said where each component had a real maximum and a real minimum. Considering those results given in Figures 9-12, it was discovered that no reasonable result could be obtained from the simulations carried out using the central difference formula approach of solving the models of the reactive packed distillation process used for

the production of ethyl acetate from the esterification reaction between acetic acid and ethanol.

Apart from using the graphical illustrations to investigate the performances of the different difference formula approaches used for the solutions of the developed models for the reactive packed distillation process, as mentioned before, a prototype plant developed using Aspen Plus was run using the same data given in Table-1 that were used to simulate the process models and the results obtained from the runs compared with those of the simulations are as given in Table-2.

**Table-2.** Measured and simulation top segment temperatures and top liquid ethyl acetate mole fractions.

Method	$T_{top}$ (°C)	$x_{EtAc}$	$T_{top}$ percentage residual (%)	$x_{EtAc}$ percentage residual (%)
Measured	349.79	0.7832	-	-
Backward difference	350.78	0.7691	0.28	1.79
Forward difference	368.66	0.0482	5.40	93.85
Central difference	358.26	0.3193	2.42	59.24

As can be seen from Table-2, among the three simulation approaches investigated in this work, the one that gave the lowest percentage residuals, calculated as the percentage of the difference between the measured and the simulation value divided by the measured value, for both the top segment temperature and the top liquid ethyl acetate mole fraction was backward difference.

#### 4. CONCLUSIONS

It has been discovered in this work that, among the three difference formula approaches employed in the solution of the dynamic models developed for the reactive packed distillation process used for the production of ethyl acetate from the esterification reaction occurring between acetic acid and ethanol, the best one was backward difference formula approach because it was able to give

the highest mole fraction of ethyl acetate obtained from the top segment of the column. Besides, its (backward difference)'s results (top ethyl acetate mole fraction and temperature) were found to compare very well with the results obtained from the developed prototype pilot plant of the process.

#### Nomenclatures

- \* Equilibrium
- a Acetic acid
- A, B, C Antoine constants
- $A_c$  Column cross sectional area ( $m^2$ )
- $A_{cat}$  Catalyst specific surface area ( $m^2/kg$ )
- cat Catalyst
- e Ethanol



F	Feed ratio (mL min <sup>-1</sup> acetic acid/mL min <sup>-1</sup> ethanol)	Pérez-Correa S. González P. and Alvarez J. 2008. On-Line Optimizing Control for a Class of Batch Reactive Distillation Columns. Proceedings of the 17 <sup>th</sup> International Federation of Automatic Control (IFAC) World Congress, Seoul, Korea. 17: 3263-3268.
fa	Acetic acid feed	
F <sub>a</sub>	Acetic acid feed molar rate (kmol/s)	
fe	Ethanol feed	
F <sub>e</sub>	Ethanol feed molar rate (kmol/s)	
h	Solution step height (m)	Sinnott R.K. 2005. Coulson and Richardson's Chemical Engineering. 4 <sup>th</sup> Edition. Elsevier Butterworth-Heinemann, Amsterdam. 6: 1045.
i	Component	
j	Column segment	
K	Phase equilibrium constant	
K <sub>eq</sub>	Equilibrium reaction rate constant	Taylor R. and Krishna R. 2000. Modelling Reactive Distillation. Chemical Engineering Science. 55: 5183-5229.
k <sub>ya</sub>	Mass transfer coefficient (kmol/(m <sup>2</sup> s))	
L	Liquid molar flow rate (kmol/s)	
M	Molar hold up (kmol)	
m	Total component number	
M'	Molar hold per segment (kmol/m)	
n	Total segment number	
p	Vapor pressure (mmHg)	
r'	Reaction rate (kmol/(kg s))	
R	Reflux ratio (kmol s <sup>-1</sup> recycled liquid / kmol s <sup>-1</sup> distillate)	
T	Temperature (K)	
t	Time (s)	
T <sub>top</sub>	Top segment temperature (K)	
V	Vapor molar flow rate (kmol/s)	
W	Catalyst weight (kg <sub>cat</sub> )	
x	An arbitrary variable, liquid mole fraction	
x <sub>EtAc</sub>	Top segment liquid ethyl acetate mole fraction	
y	Vapor mole fraction	
z	Flow length (m)	

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