MATHEMATICAL MODEL FOR MULTICOMPNENT DISTILLATION COULOM

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ABSTRACT

A mathematical model of a distillation column has been carried out for an existing distillation column in a phenol plant.The developed mathematical model for the distillation column was encountered with the high nonlinearty of the system considering the material and energy balances and the highly time lag within the column. The model of distillation column was simulated on a personal computer using Newton-Raphson method for nonlinear algebraic equations solution, the results obtained were reliable.

A comparison between present method and Gear method has been carried out, and the results show that the model has high accuracy

INTRODUCTION

There has been a continuous development for dynamic model of the distillation column and fast approximate in strategies for the maintaining product specifications.

Generally the dynamic studies depend on the theory and equations that are used to represent the distillation column. Also, the used computation technique for solving the model equations is a very important factor in the model body.

Tyreus et al.(1975), Ballard and Brosilow (1978) and Gallun and Holland (1982) modeled distillation column accounting for variation in liquid holdup and some other tray hydraulic parameters using a Semi-Implicit Rung Kutta (SIRK) method and Gear's method respectively, moreover, their results analyzed with the use of industrial data to get efficient results which were compared with other simple hydraulic models.

Prokopakis and Seider (1983) generated a new algorithm for the integration of the material balance, equilibrium, summation of mole fraction and heat balance equations (MESH) using the adaptive semi-implicit Rung-Kutta (ASIRK) integrator that appears to be efficient and reliable for simulation of azeotropic distillation configurations. The dynamic of the decanter are modeled separately, then combined with the MESH equations group.

Hess et al. (1981) used a technique that divides the distillation column into any arbitrary number of sub units in which the equations for the sub units are solved sequentially. The good convergence characteristics exhibited by the proposed methods can be attributed to the fact that the proposed procedure may be reduced either to exact methods or to the methods that are nearly exact in certain limiting cases.

Beenallou et al. (1986) developed a low-order modeling technique for separation processes by considering a staged column as a compartment in which the number of stages is lumped to form an equivalent stage. This method leads to a low-order method of separation processes directly and without linearization. This model provides acceptable result with distillation column as a part of separation processes.

Gani et al. (1986) presented a generalized model for the dynamic simulation of distillation columns. The successful application of the model to solve different type of test problems demonstrated its wide applicability and flexibility. The good matching of the industrial data showed that the model was reliable and could be used for the study of industrial processes. Even where the industrial data were not available, the quantitative analyses of the results obtained seemed to be very reasonable.

Cameron et al. (1986) presented numerical and computational aspects related to the solution of Gani et al. (1986) model. The algorithm has proved extremely reliable and robust in the solution of distillation dynamic problems. For low-accuracy requirement (local error tolerance 10^{-3} - 10^{-4}), the Diagonally Implicit Rung Kutta (DIRK) code was efficient and extremely robust.

At higher accuracies the Backward-Differentiation (BDF) code becomes preferable.

Jacobsen et al. (1991) showed that the multiplicity of the distillation column depend on the assumption, number of streams, number of component, vapor liquid equilibrium relation, mean theory and equations used to represent the distillation column.

Wijn (1998) stated that the lower range of operation can be recognized into three conditions:

At rates below the seal point (the damping range), both gas and liquid flow through the perforated area of the tray and no liquid flows through the downcomer. The hydraulic behavior has become equivalent to that of a try without downcomer (a dual flow tray).

Between weeping point and seal point (the weeping range), the liquid flow switches from flow across the tray to a condition of countercurrent flow through the perforations.

At gas rates in excess of the weep point (the normal operating range), the perforations are utilized by the gas flow exclusively. The inlet liquid flow rate is transported over the outlet weir and through the downcomer.

Wijn (1998) described a model that gives liquid height and weep fraction as a function of gas and liquid flow rates for a given tray layout.

THE MATHEMATICAL MODEL

Realistic performance of an essential operation and actual column can seldom be predicted satisfactorily by excluding the simultaneous effects of heat and mass transfer and fluid flow on the trays. Tray hydraulics is an important factor in predicting the dynamic performance, because of its effect on heat and mass transfer calculations. Accurate prediction of physical properties is also important.

A generalized model should takes into consideration all the factors and variables that describe the process, and would be numerically robust, efficient in terms of computing time and storage even for very large industrial problems. Also the model would be flexible enough to allow the study of a wide or significant application both in terms of research and development as well as solving practical problems.

Assumptions

Seven assumptions made in the development of the proposed model:

1. The molar vapor holdup is negligible compared to the molar liquid hold-up.
2. The liquid and vapor leaving each tray are in thermal equilibrium.
3. Liquid and vapor are totally mixed on each tray.
4. Liquid and vapor entrainment is ignored in calculation procedure.
5. A vapor in the column is handled with ideal gas behavior .
6. Heat losses are neglected.
7. Constant tray efficiency along distillation column.

First assumption is quite reasonable since in most systems, the vapor density is considerably smaller than the liquid density. The assumption of totally mixing is necessary to reduce the complexity of the problem. Models of mixing on plates are very complex and involve partial differential equations. Similarly, more accurate efficiency models are very complex. The accuracy that can be achieved with these complex models at the expense of the dimension of the problem and computing time was considered. Satisfactory correlation for entrainment flow rate calculation did not found yet, so assumption four is given. Assumption six is widely used because of the complexity of heat transfer equations. Final assumption is used especially to examine the system because of its abnormal operation as mentioned above.

Fundamentals and Equations of the Model

With above objectives in mind, the proposed generalized model has been developed. That's development based on the solution of non-linear dynamical model.

The model consists of a set of ODEs that obtained from the mass and energy balances around each tray of the distillation column, in addition the reboiler and the condenser. Moreover, a set of algebraic equations/ correlation's which are used to predict the physical properties, tray hydraulic, mass transfer rate and dynamic function for reflux drum and reboiler. The variables that appear on the ODEs will be termed "differential" variables, all other variables except time will be termed as "algebraic" variables, that will be the independent variable.

Mass and Energy Balances

1. The total mass balance around tray p is equal to:

$$\frac{dm_p}{dt}=F_p^V+F_p^L+V_{p-1}+L_{p+1}-W_p+S_p^V-V_p-S_p^L-L_p \quad (1)$$

2. Component mass balance around tray p for component i:

$$\frac{d(m_p\cdot x_{p,i})}{dt}=F_p^V\cdot y_{p,i}^f+F_p^L\cdot x_{p,i}^f+V_{p-1}\cdot y_{p-1,i}+L_{p+1}\cdot x_{p+1,i} \\ -W_p\cdot x_{p+1,i}-(S_p^V+V_p)y_{p,i}-(S_p^L+L_p)x_{p-1,i} \quad (2)$$

3. Total energy balance around tray p:

$$\frac{d(m_p\cdot h_p)}{dt}=F_p^V\cdot H_p^f+F_p^L\cdot h_p^f+V_{p-1}\cdot H_{p-1}+L_{p+1}\cdot h_{p+1}-W_p\cdot h_{p+1} \\ -(S_p^V+V_p)H_p-(S_p^L+L_p)h_{p-1} \quad (3)$$

Vapor Liquid Equilibrium Correlation

1. Composition of vapor stream on each tray can be predicted using the following equilibrium relation:

$$y_{p,i}^{*}=K_{p,i}\cdot x_{p,i} \quad (4)$$

2. The equilibrium factor $K_{p,i}$ was calculated using the following equation:

$$K_{p,i}=\frac{\gamma_{p,i}\cdot P_{p,i}^{*}}{\varphi_p\cdot P_p^T} \quad (5)$$

3. The two variables $(\gamma_{p,i}\ \&\ \varphi_{p,i})$ are defined as a correction factor for liquid and vapor ideality respectively, named activity and fugacity coefficients.

The calculation of activity coefficient using UNIFAC method was elucidated in Smith (1986) with details that will be used in the present work. Fugacity coefficient is taken as unity because the distillation column is operating in low pressure.

Tray Efficiency

The Murphree plate efficiency (Murphree, 1925) which is defined as:

$$Me_p=\frac{y_{p,i}-y_{p-1,i}}{y_{p,i}^{*}-y_{p-1,i}} \quad (6)$$

That was used in the present work, and the efficiency measured directly from the phenol plant, by measuring the column efficiency and then applied it as tray efficiency.

Tray Hydrodynamic Correlation

Most correlations attribute total pressure drop to three factors, these factors are the clear liquid height on the tray, the passage of the vapor through the perforations, and the formation of vapor bubbles. It has been customary to express pressure drop in terms of height of liquid on the tray (Bennett, 1983).

Molar Holdup

Molar holdup on tray is function to many parameters. Gani (1986) suggest a new correlation that is utilized for distillation modeling.

Moreover, definition of liquid holdup on tray, Gani et al. (1986) defined the molar liquid holdup on tray as the summation of molar weight over the plate and molar liquid weight in the downcomer, because they have the same concentration and physical properties

$$m_p=m'_p+m_p^D \quad (7)$$

Mass and Energy Balance around Reboiler and Condenser

1. Total mass balance around reboiler is:

$$\frac{dm_1}{dt}=L_2-V_1-L_1 \quad (8)$$

2. Component mass balance around reboiler is:

$$\frac{d(m_1\cdot x_{1,i})}{dt}=L_2\cdot x_{2,i}-V_1\cdot y_{1,i}-L_1\cdot x_{1,i} \quad (9)$$

3. Energy balance around boiler is:

$$\frac{d(m_1 \cdot h_1)}{dt} = Q_B + L_2 \cdot h_2 - V_1 \cdot H_1 - L_1 \cdot h_B \qquad (10)$$

4. Total mass balance around condenser is:

$$\frac{dm_{N_p+1}}{dt} = V_{N_p} - V_{N_p+1} - L_{N_p+1} \qquad (11)$$

5. Component mass balance around condenser is:

$$\frac{d(m_{N_p+1} \cdot x_{N_p+1,j})}{dt} = V_{N_p} \cdot y_{N_p,j} - V_{N_{P+1}} \cdot y_{N_{P+1},j} - L_{N_{P+1}} \cdot x_{N_{P,j}} \qquad (12)$$

6. Energy balance around condenser is:

$$\frac{d(m_{N_p+1} \cdot h_{N_p+1})}{dt} = Q_C + V_{N_p} \cdot H_{N_p} - V_{N_p+1} \cdot H_{N_{P+1}} - L_{N_p+1} \cdot h_{N_p+1} \qquad (13)$$

Equations and Constraints

Additional equations were needed to complete the model, there are:

1. The error in the summation of vapor and liquid fractions :

$$\sum_{i=1}^{nc} x_{p,i} - 1 = \sum_{i=1}^{nc} y_{p,i} - 1 = 0 \qquad (14)$$

2. The difference between evaluated and calculated heat enthalpy for liquid holdup defined as error in enthalpy.

$$H_p^{Cal} - H_p^{Eva} = 0 \qquad (15)$$

3. Where H_p^{Eva} are evaluated from the integration of the ODEs of energy balance and finally:

$$H_P^{Cal} = \int_{T_{ref}}^{T_P} m_P \cdot C_P^L \cdot dT \; (C_P^L = a + b \cdot T + c \cdot T^2) \qquad (16)$$

Composite Matrices Description

The matrices result from the present model are combination of more than one type. This section discusses and describes these matrices with details.

1. Ordinary differential equations matrix.

$$\begin{array}{ccl}
R = & \left[\begin{array}{cccccccc}
r_{1,1} & r_{1,2} & r_{1,3} & r_{1,4} & r_{1,5} & \cdots & \cdots & r_{1,N} \\
r_{2,1} & r_{2,2} & r_{2,3} & r_{2,4} & \cdots & \cdots & \cdots & \cdots \\
r_{3,1} & r_{3,2} & r_{3,3} & \cdots & \cdots & \cdots & \cdots & \cdots \\
r_{4,1} & r_{4,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
r_{5,1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & r_{i,j} & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
r_{n+2,1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & r_{n+2,N}
\end{array}\right] & \begin{array}{l}
\leftarrow \text{Total M.B} \\
\leftarrow \text{Total E.B} \\
\left.\begin{array}{l} \\ \\ \\ \\ \\ \\ \end{array}\right\} \text{Conc. M.B}
\end{array} \\
 & \begin{array}{lr} \uparrow \qquad\qquad\qquad\qquad\qquad\qquad & \uparrow \\ \text{Boiler} \qquad\qquad\qquad\qquad\qquad\qquad & \text{Condenser} \end{array} &
\end{array} \qquad (17)$$

2. Differential variables matrix.

As shown later, the variables that appear on the ODEs well be termed "differential" variables these variables are combined to generate matrix Y that is described as:

$$\begin{array}{ccl}
Y = & \left[\begin{array}{cccccccc}
Y_{1,1} & Y_{1,2} & Y_{1,3} & Y_{1,4} & \cdots & \cdots & \cdots & Y_{1,N} \\
Y_{2,1} & Y_{2,2} & Y_{2,3} & Y_{2,4} & \cdots & \cdots & \cdots & \cdots \\
Y_{3,1} & Y_{3,2} & Y_{3,3} & \cdots & \cdots & \cdots & \cdots & \cdots \\
Y_{4,1} & Y_{4,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & Y_{i,j} & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
Y_{n+2,1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & Y_{n+2,N}
\end{array}\right] & \begin{array}{l}
\leftarrow \text{Liquid holdup} \\
\leftarrow \text{Liquid enthalpy} \\
\left.\begin{array}{l} \\ \\ \\ \\ \\ \\ \end{array}\right\} \begin{array}{l} \text{Trays holdup} \\ \text{Concentration} \end{array}
\end{array} \\
 & \begin{array}{lr} \uparrow \qquad\qquad\qquad\qquad\qquad\qquad & \uparrow \\ \text{Boiler} \qquad\qquad\qquad\qquad\qquad\qquad & \text{Condenser} \end{array} &
\end{array} \qquad (18)$$

3. Algebraic variables matrix:

This matrix combined the residual variables termed "algebraic" variables.

$$\begin{array}{ccl}
Z = & \left[\begin{array}{cccccccc}
z_{1,1} & z_{1,2} & z_{1,3} & z_{1,4} & z_{1,5} & \cdots & \cdots & z_{1,N} \\
z_{2,1} & z_{2,2} & z_{2,3} & z_{2,4} & \cdots & \cdots & \cdots & \cdots \\
z_{3,1} & z_{3,2} & z_{3,3} & \cdots & \cdots & \cdots & \cdots & \cdots \\
z_{4,1} & z_{4,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
z_{5,1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & z_{i,j} & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
z_{n+4,1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & z_{n+4,N}
\end{array}\right] & \begin{array}{l}
\leftarrow \text{Vapor flow rate} \\
\leftarrow \text{Liquid flow rate} \\
\leftarrow \text{Pressure} \\
\leftarrow \text{Temperature} \\
\left.\begin{array}{l} \\ \\ \\ \\ \end{array}\right\} \text{Vapor Concentration}
\end{array} \\
 & \begin{array}{lr} \uparrow \qquad\qquad\qquad\qquad\qquad\qquad & \uparrow \\ \text{Boiler} \qquad\qquad\qquad\qquad\qquad\qquad & \text{Condenser} \end{array} &
\end{array} \qquad (19)$$

4. Non-linear dynamic function.

The gathering of the hydrodynamic, vapor liquid equilibrium and constrains equations generates a composite matrix function that is G, these equations Solved simultaneously to get matrix Z which is defined above.

$$\begin{array}{ccl}
G = & \left[\begin{array}{cccccccc}
g_{1,1} & g_{1,2} & g_{1,3} & g_{1,4} & \cdots & \cdots & \cdots & g_{1,N} \\
g_{2,1} & g_{2,2} & g_{2,3} & g_{2,4} & \cdots & \cdots & \cdots & \cdots \\
g_{3,1} & g_{3,2} & g_{3,3} & \cdots & \cdots & \cdots & \cdots & \cdots \\
g_{4,1} & g_{4,2} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & g_{i,j} & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
g_{n+4,1} & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & g_{n+4,N}
\end{array}\right] & \begin{array}{l}
\leftarrow \text{Hydrodynamic (L)} \\
\leftarrow \text{Hydrodynamic (V)} \\
\leftarrow \text{Sum. of vapor conc.} \\
\leftarrow \text{Enthalpy error} \\
\left.\begin{array}{l} \\ \\ \\ \\ \end{array}\right\} \text{Equilibrium relation}
\end{array} \\
 & \begin{array}{lr} \uparrow \qquad\qquad\qquad\qquad\qquad\qquad & \uparrow \\ \text{Boiler} \qquad\qquad\qquad\qquad\qquad\qquad & \text{Condenser} \end{array} &
\end{array} \qquad (20)$$

Formulation of Dynamic Model

The dynamic model is constructed using above medley matrices to simulate the distillation column operation. This transfer function can be described by. the relation between Y&X can be expressed as:

$$Y = \int_0 R' \cdot dt \tag{21}$$

The solution method used is the Euler method for differential equations and Newton-Raphson method for algabric equations as follows.

$$Y_{n+1} = Y_n + \left(R'_{t+\Delta t} - R'_t\right) \cdot \Delta t \tag{22}$$

Where R' is a combination of ordinary differential equations matrix, and Y is the differential variables or the solution of the differential variables. In addition, the integration method is the Euler method (Shinskey 1967).

Moreover, the calculation of matrix R' will be as follows:

- R' (t=0), Steady state analysis. This analysis depends on setting ODEs equal to zero. Then solved as a matrix of algebraic equations using iterative method.
- R' (t>0) = acceptable solution of the G equation using iterative method.

Newton-Raphson with Method Matrix Equations

In the widespread case Newton-Raphson method applied to set of equations that formed as vector. Nevertheless, if the sets of nonlinear equations formed as matrix, the derivation of the main equations and its structures remain without changes in details but in its component as follow:

$$[\bar{x}] = [x] - [J]^{-1}\{f\} \tag{23}$$

Where: $\bar{x}$ = New value of solution matrix, x = previous value of solution matrix, f = function matrix, J = Jacobian matrix, and Keep in mind where f vector:

$$J_{i,j} = \frac{\partial f_i}{\partial x_j} \tag{24}$$

But if f matrix then: $J_{i,j,k,l} = \dfrac{\partial f_{i,j}}{\partial x_{k,l}}$ (25)

RESULTS AND DISCUSSION

The computer simulation is first run to obtain a steady state column profile. The Steady state characteristics are important to be the initial condition for transient response simulation. The simulation software is written using (Visual C++ 6, 1999).

Using Gallun (1982) test column to predict the accuracy of the model and the way of solution, Table (1) shows the comparison between the recent model and Gear model, the results are in agreement with that of previous work.

Also Table (1) shows the effect of the hydrodynamic correlation that express the pressure drop in terms of height of liquid on tray, the used correlation gave almost identical pressure drop and reflux ratio to that of reality.

The model is also tested on a phenol plant distillation column, which separates benzoic acid/ phenol/ water mixture. In steady state condition, the top product is nearly water-phenol mixture and bottom product is nearly benzoic acid only.

Open loop test completed by 10% step change in vapor boilup, feed flow rate and concentration and reflux flow rate. Figures (1-3) show transient response for test column, that appear good and reasonable compared with common distillation column.

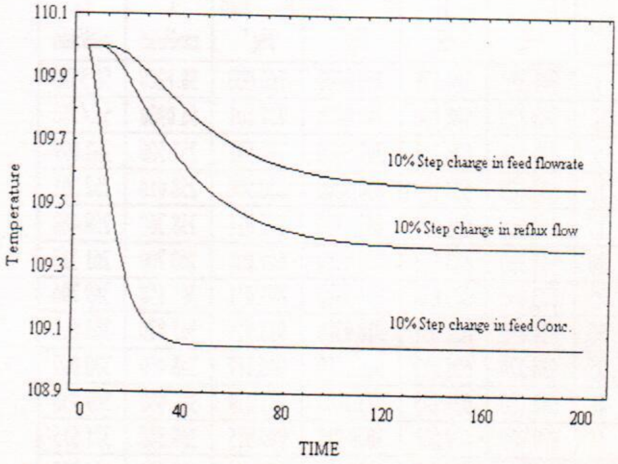

Fig. 1 The effect of different step changes on top temperature

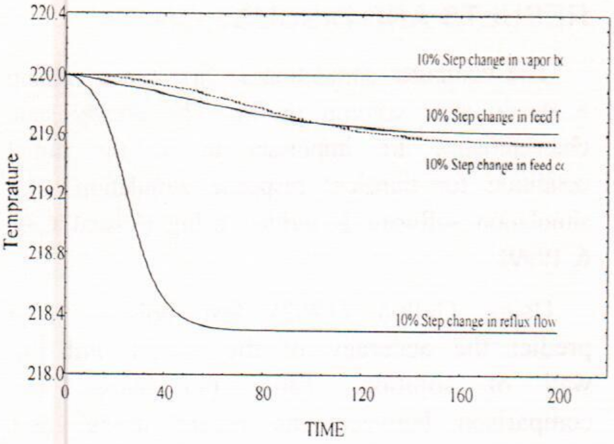

Fig. 2 Effect of different step changes on bottom tempeature

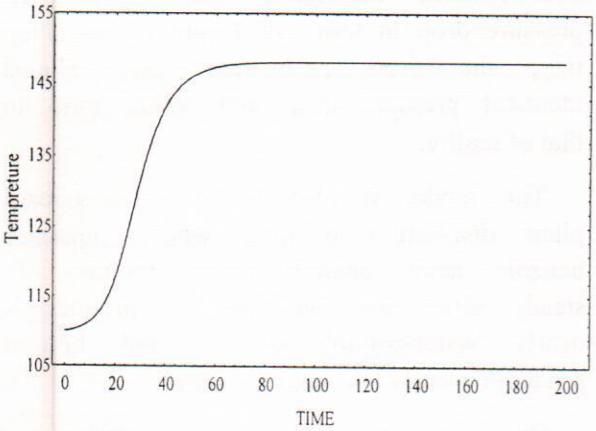

Fig. 3 Effect of 10% vapor boilup step changes on the top temperature

Table 1 characteristic data of Gallun compared with present results

No.	T °R	T_1 °R	P mm Hg'	P_1 mm Hg'	L mol/min	L_1 mol/min
1	594.370	594.171	760.0000	760.000	58.1200	58.5570
2	598.320	598.130	787.0900	787.101	56.0900	56.4750
5	626.840	626.718	797.5900	797.581	257.500	258.899
10	633.060	633.103	820.5200	820.580	258.010	258.201
15	635.600	636.655	842.9800	842.911	258.360	259.488
20	633.230	633.133	865.0100	867.000	260.700	261.226
25	623.000	623.018	891.5700	891.011	367.150	369.706
30	624.630	624.651	918.9300	918.955	367.820	368.888
35	626.220	626.212	946.1600	946.117	368.460	370.069
40	627.800	627.795	973.2800	973.219	369.080	369.938
45	629.900	629.881	1000.210	999.515	369.380	371.515
50	645.240	645.195	1025.550	1025.15	235.000	236.252

Continued from Table 1

No.	V mol/min	V_1 mol/min	m moles	m_1 moles	m*h Btu*10^{-3}	m_1*h_1 Btu*10^{-3}
1	...	...	281.290	281.682	831280	832447.4
2	81.370	81.696	19.710	19.885	58540	58665.0
5	72.390	73.302	71.390	71.486	186830	187095.2
10	72.910	74.665	72.270	72.722	196780	196993.7
15	73.290	74.565	72.770	73.738	200320	200769.5
20	74.180	75.895	73.800	73.851	198390	198703.3
25	82.010	82.399	84.370	85.448	222180	222406.7
30	82.680	83.374	84.480	84.830	225420	226035.5
35	83.330	83.702	84.590	84.865	228580	228992.0
40	83.960	86.049	84.690	85.620	231670	231786.9
45	84.410	85.375	84.770	85.267	234900	235151.2
50	82.180	84.230	3494.91	3505	10236900	10240800

CONCLUSIONS

From the present work, it was concluded that:

1. From the results obtained, the proposed model was reliable and more flexible to study different, difficult and multiple columns.
2. The open loop behaviors of the column to disturbance were acceptable except that for a step change in the vapour from the boiler which made the temperature of the condenser to rise up (specially at temperature =145 °C). This behavior will lead to the freezing of the benzoic acid in the condenser tubes and valves.

NOMENCLATURE

Symbol	Description	Unit
F_p^L	Liquid feed flow rate to tray (p)	Kg mole/hr
F_p^V	Vapor feed flow rate to tray (p)	Kg mole/hr
H_p	Liquid enthalpy at tray (p)	KJ/Kg mole
H_p	Vapor enthalpy at tray (p)	KJ/Kg mole
K_{pi}	Liquid – vapor equilibrium constant	-
L_p	Liquid flow rate from plat (p)	Kg mole/hr
M_p	Total molar holdup on tray (p)	Kg mole
$M_{p'}$	Total molar over the plat (p)	Kg mole
M_p^D	Total molar in the downcomer (p)	Kg mole
S_p^L	Liquid side stream flow rate at plate (p)	Kg mole/hr
S_p^V	Vapor side stream flow rate at plate (p)	Kg mole/hr
T	Time	Hr
V_p	Vapor flow rate from plat (p)	Kg mole/hr
W_p	Weeping flow rate from plat (p)	Kg mole/hr
X_{pi}	Liquid mole fraction of component (i) at tray (p)	-
Y_{pi}	Vapor mole fraction of component (i) at tray (p)	-
ρ_p^L	Density of liquid leave the plate (p)	Kg mole/m^3
ρ_p^V	Density of vapor leave the plate (p)	Kg mole/m^3

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