DYNAMIC MODELLING AND SIMULATION OF MULTIVESSEL BATCH DISTILLATION COLUMN

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ABSTRACT

Traditionally, the separation of multicomponent mixtures by using batch distillation column, is accomplished by collecting the product at the top one after the other and recycling the off-cuts. Hasebe et al (1995) and Skogestad et al (1995), proposed an alternative design of batch distillation column. In this paper, a dynamic model of this new design was developed and simulation experiments were performed. The results indicate that the multivessel batch distillation column is feasible to operate. By using control scheme proposed by Skogestad et al (1995) the final composition in the vessels at infinite time (steady state) does not depend on feed characteristics.

INTRODUCTION

The batch distillation process mostly is found in situation where feeds change from batch to batch and where distillation is required at irregular intervals. Also, when the production of purest products from a multicomponent mixture is required.

Multicomponent batch distillation is becoming increasingly important as a result of the expansion of fine and specialty chemicals as well as pharmaceutical products industries. These industries are characterized by small amounts of products with high added value and greater demand for flexibility and productivity. Environmental protection which needs the recovery of profitable and toxic materials and development of advanced techniques in process control are also, the reasons for increase in popularity of multicomponent batch distillation.

Therefore, the availability of a practicable technique for developing effective and reliable operation of multicomponent batch distillation is very important. There are a number of researches dealing with multicomponent

batch distillation, but mostly restricted to separate a multicomponent mixture into its components by sequence of N-1 operations, which proves to be energy intensive.

A new strategy for separating multicomponent mixtures simultaneously was first proposed by Hasebe et al (1995) and Skogestad et al (1995). The feature of the system is that it contains only one reboiler, (N-1) vessels, (N-1) column sections and single condenser (see Fig. 1 below). This type of column is known as multivessel batch distillation column.

With N vessels (including the reboiler) and (N-1) column sections, it is possible to separate N components into their purest form. The advantage with this multivessel batch column compared to regular batch distillation column, where the products are collected over at the top one at time, is that the off-cuts and separation of these can be avoided.

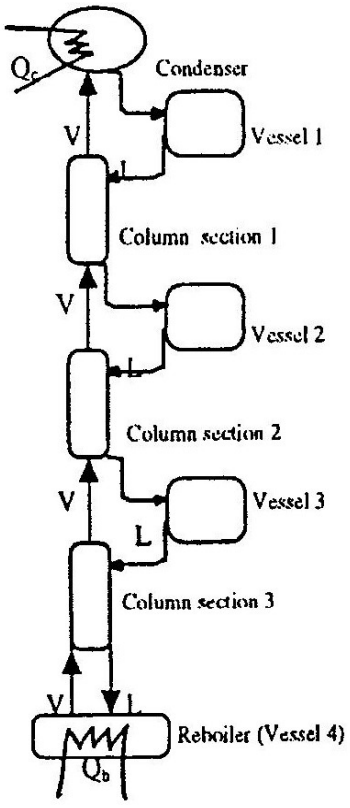


Fig. 1: Flowsheet of multivessel batch distillation column

MODELLING

The mathematical modelling of a process, as defined by Denn (1986), is a system of equations whose solution, given specified input data, is representative of the response of the process to corresponding sets of inputs. The dynamic process models are, usually, obtained by using fundamental principles, possibly combined with parameter fitting to match observations of the real process. Empirical models obtained from observations only generally are used for smoothening data. This approach may not safely be used to predict the behaviour of the system at other operating conditions.

In chemical engineering, process models are used for several purposes. These includes process and/or equipment design, process optimization, process monitoring, operator training, process control and establishing procedure for start-up and shutdown or handling troubleshooting. Thus, dynamic modelling is very useful for chemical engineers in obtaining insight and understanding of the process.

The model of distillation column usually refers to a stage model that includes mass - and energy - balance on each stage, liquid flow dynamics, pressure dynamics, pressure dynamics and detail of reboiler and condenser. Such mode is complex and difficult to work with. The level of modelling is an important issue. There are a number of reasons why one should try to keep a model as simple as possible. Using a simple model makes it easier to understand, avoids errors and saves time. In addition, there are two fundamental reasons of using simplified model, namely:

i) If the model is too complex then it may be unsolvable with the available computing power

ii) It may require a large number of parameters values which may not be available from independent sources.

Although the art of modelling may be formalized to some degree, the results will nevertheless depend strongly on the experience and intuition of the engineer.

The art is to make a simple, yet sound model by making the appropriate simplifications and assumptions using incomplete data. Some typical assumptions include assuming perfect mixing in both phases in all stages,

thermal and thermodynamic equilibrium between phases and neglecting the effect of column internals on the energy balance.

The model developed for staged column can also be used in packed column. Though packed column can be modeled by using partial differential equations, it has been proved (Skogestad (1992) that the packed column can be well modeled by using staged model with estimated number of stages obtained from correlation or observations of the real column. Stage models are used for numerical reasons and also because it is dificult to obtain mass transfer data, etc. needed for packed column model.

MATHEMATICAL MODEL OF MULTIVESSEL BATCH DISTILLATION COLUMN

The mathematical model for the multivesel batch distillation column is based on the model of a regular batch distillation column. The proposed model is based on the following assumptions:

i) constant volatility
ii) constant molar liquid and vapour flow (neglect flow dynamics)
iii) constant pressure
iv) constant molar hold-up on trays
v) constant efficiency (100%)
vi) negligible vapour hold-up
vii) total condenser
viii) perfect mixing on all trays and in all vessels.

The multivessel distillation column is modeled as a stack of stages (counted from top) where the tray hold up is kept constant. The interconnection of tray and vessels is shown in Fig. 2.

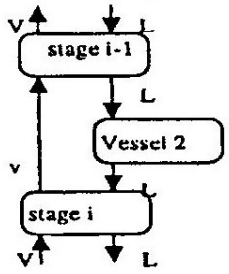


Fig. 2: Tray and vessel interconnection

The model for tray i consists of a component mass balance

$$M_i \frac{dx_{ji}}{dt} = L(x_{ji-1} - x_{ji}) + V(y_{ji+1} - y_{ji}) \quad (1)$$

Due to the constant relative volatility assumption and negligible vapour hold-up, the energy balance is neglected. The vapour - liquid equilibrium is given by the following equation.

$$\alpha_{jz} = \frac{y_j / x_j}{y_z / x_z} \quad (2)$$

where
j = 1,2,3,4 (component number)
z = 1,2,3,4 (component number)

The model of the intermediate vessels is given by the mass balance as:

$$\frac{d(M_v x_{jv})}{dt} = L(x_{ji} - x_{jv}) \quad (3)$$

and the modelling of the condenser (note that it is assumed a total condenser), the mass balance is;

$$M_c \frac{dx_{jc}}{dt} = Vy_{ji} - Lx_{jc} \quad (4)$$

Note that the vapour flow does not pass through the vessels or the condenser, such that an equilibrium calculation is not necessary.

The reboiler is modeled by the following equation:

$$\frac{d(M_r x_{jr})}{dt} = Lx_{jw} - Vy_{jr} \quad (5)$$

where the vapour liquid equilibrium is described by equation 2 above. the mathematical description of the reboiler is simplified by assuming a constant molar boil-up rate.

SIMULATION

In general the stage by stage model of multivessel batch distillation column

outlined above, describes the real column setup very well. The number of stages in each column section is taken to be equal for simplicity reason, and the parameters for flow dynamics are obtained from literature. The dynamic model is implemented in the SPEEDUP simulation environment (speedup,1993). The control structure implemented consists of three P-controllers which adjust the reflux to the column sections, based on the temperature in the middle of the column section below it, as proposed by Skogestad et al (1995).

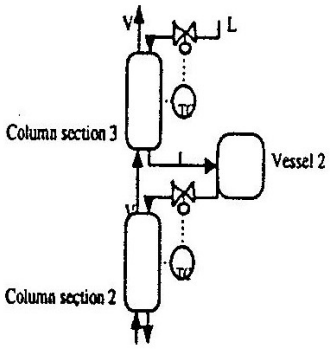


Fig. 3: Temperature control scheme of multivessel batch distillation

A series of dynamic simulations were performed to verify and study the operating capability of multivessel batch distillation column. After feeding a prescribed amount of feed to the system, total reflux operation was carried out until the composition in all vessels reach a steady state values. In the experiments done, the system was tested first, with feed distributed equally in all four vessels and secondly, most of the feed was charged in the reboiler and a very small amount distributed equally in other vessels. Table 1,2 and 3 show data and other parameters as used in the experimentation.

Table 1: summary data of the System and initial conditions

	All Experiment Run
Number of components	4
Feed composition	x_0, x_0, x_0
Relative volatility	[10.2, 4.5, 2.3, 1.0]
Number of column sections	3
Total feed [Kmols]	10.33
Tray hold-up [Kmols]	0.01
Flow [Kmols/hr]	L=10 V=10

Components used in the experiments are methanol, Ethanol, n-propanol, n-butanol

Table 2: summary of parameters used in each experimental run

	Experiment A			Experiment B			Experiment C			Experiment D		
	A1	A2	A3	B1	B2	B3	C1	C2	C3	D1	D2	D3
Feed composition	x_{f1}	x_{f2}	x_{f3}	x_{f1}	x_{f2}	x_{f3}	x_{f1}	x_{f2}	x_{f3}	x_{f1}	x_{f2}	x_{f3}
Total number of stages	18	18	18	18	18	18	33	33	33	33	33	33
Number of stages per section	6	6	6	6	6	6	11	11	11	11	11	11
Initial vessel hold-up [Kmols]	2.5	2.5	2.5	0.5	0.5	0.5	2.5	2.5	2.5	0.5	0.5	0.5

Table 3: Feed compositions used in the experiments

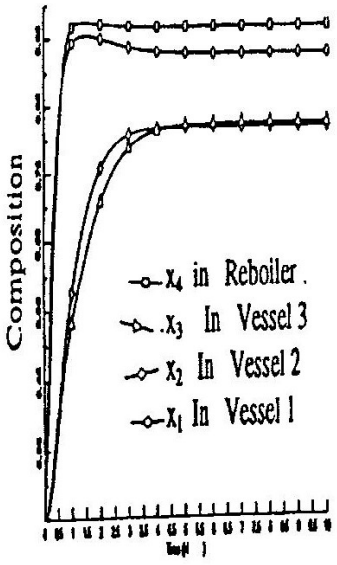
Feed	Methanol	Ethanol	n-Propanol	n-Butanol
x_{f1}	0.2500	0.2500	0.2500	0.2500
x_{f2}	0.0956	0.2570	0.1368	0.5106
x_{f3}	0.5122	0.0758	0.1186	0.2935

SIMULATION RESULTS

For reason of comparison, the simulation results with varying feed distribution in the vessels, the initial conditions for both simulations are identical and given in table 1,2 and 3 above. The controls of the reflux flow give an implicity control of the vessel hold-up, such that a desired composition of the main components in each vessels attained. The final composition in the vessels is presented in table 4 to table 15. The composition profile of main products and main impurities, are shown in Fig. 4 - 27.

Table 4:Simulation results of Experiment A1, distillation time is 8.5 hours,

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	2.417	0.0000	0.0000	0.0344	0.9655
Vessel B	2.595	0.0001	0.1100	0.8222	0.0677
Vessel C	2.466	0.0748	0.8164	0.1088	0.0001
Vessel D	2.522	0.9254	0.0745	0.0002	0.0000



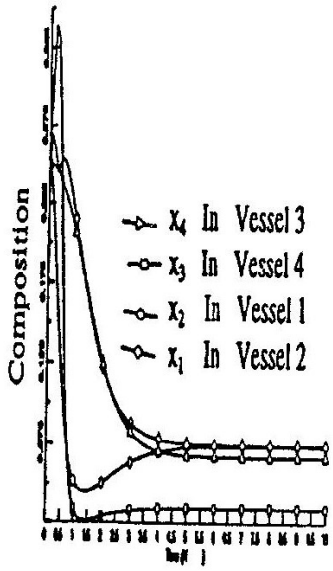
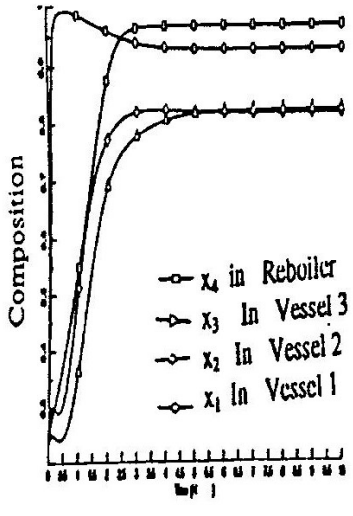


Fig 4 Main product experiment A1 Fig. 5: Main impurity experiment A1

Table 5: Simulation results of experiment B1, distillation time is 9.5 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	2.417	0.0000	0.0000	0.0344	0.9655
Vessel B	2.595	0.0001	0.1100	0.8222	0.0677
Vessel C	2.466	0.0748	0.8164	0.1088	0.0001
Vessel D	2.522	0.9254	0.0745	0.0002	0.0000



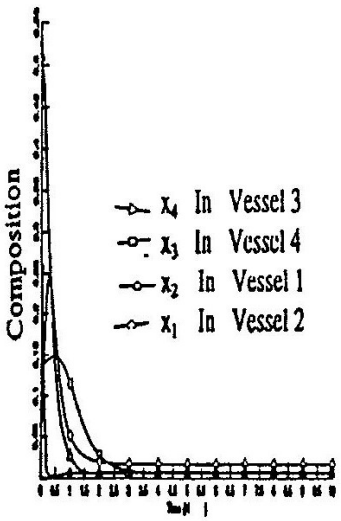
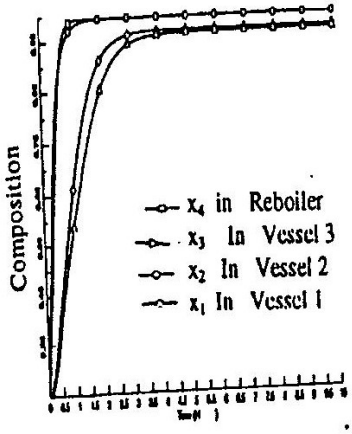


Fig. 6: Main product experiment A1 Fig. 7: Main impurity experiment B1

Table 6: Simulation results of experiment C1, distillation time is 6.5 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	2.530	0.0000	0.0000	0.0070	0.9930
Vessel B	2.512	0.0000	0. 0335	0.9603	0.0062
Vessel C	2.452	0.0162	0.9666	0.0172	0.0000
Vessel D	2.506	0.9927	0.0073	0.0000	0.0000



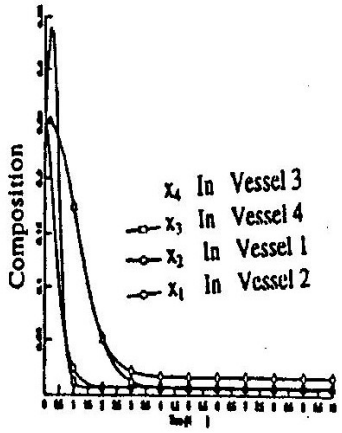
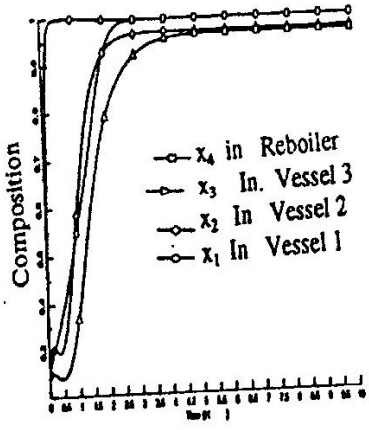


Fig. 8: Main product experiment D1 Fig. 9: Main impurity experiment C1

Table 7: Simulation results of experiment D1, distillation time is 7.1.5 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	2.530	0.0000	0.0000	0.0070	0.9930
Vessel B	2.512	0.0000	.0. 0335	0.9603	0.0062
Vessel C	2.452	0.0162	0.9666	0.0172	0.0000
Vessel D	2.506	0.9927	0.0073	0.0000	0.0000



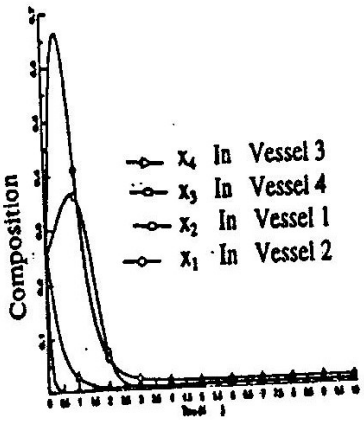
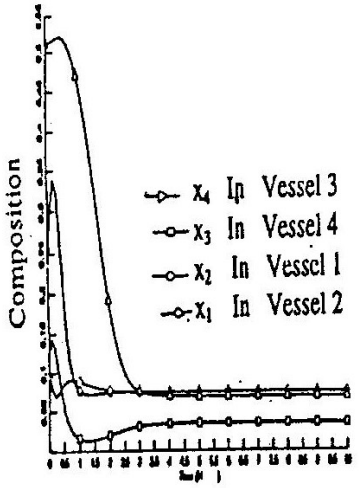


Fig. 10: Main product experiment D1 Fig. 11: Main impurity experiment D1

Table 8: Simulation results of experiment A2, distillation time is 7.0 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.276	0.0000	0.0000	0.0344	0.9655
Vessel B	1.013	0.0001	0.1100	0.8222	0.0677
Vessel C	2.924	0.0748	0.8164	0.1088	0.0001
Vessel D	0.786	0.9254	0.0745	0.0002	0.0000



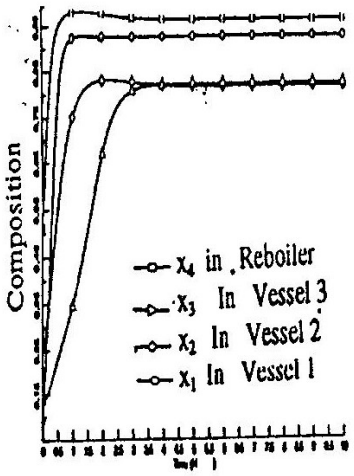
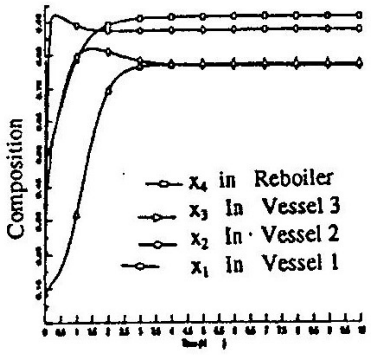


Fig. 12: Main product experiment B2 Fig. 13: Main impurity experiment A2

Table 9: Simulation results of experiment B2, distillation time is 8.0 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.276	0.0000	0.0000	0.0344	0.9655
Vessel B	1.013	0.0001	0.1100	0.8222	0.0677
Vessel C	2.924	0.0748	0.8164	0.1088	0.0001
Vessel D	0.787	0.9254	0.0745	0.0002	0.0000



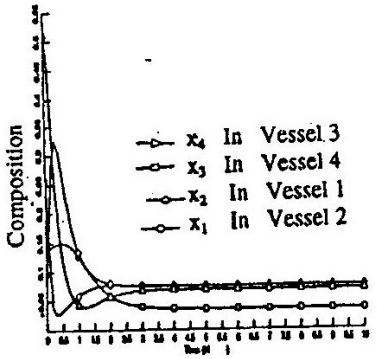
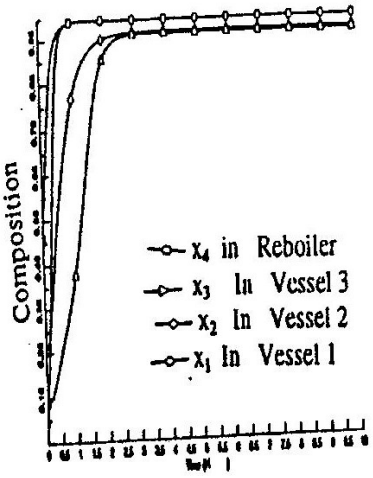


Fig. 14 Main product experiment B2 Fig. 15: Main impurity experiment B2

Table 10: Simulation results of experiment C2, distillation time is 5.5 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.249	0.0000	0.0000	0.0070	0.9930
Vessel B	1.272	0.0000	0. 0335	0.9603	0.0062
Vessel C	2.582	0.0162	0.9666	0.0172	0.0000
Vessel D	0.897	0.9927	0.0073	0.0000	0.0000



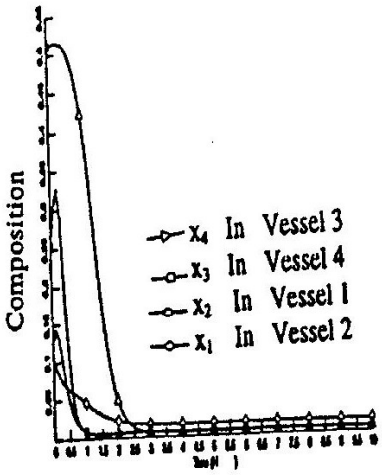
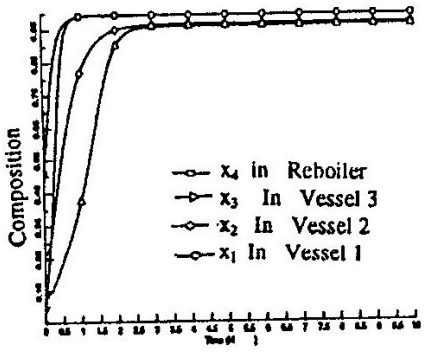


Fig. 16: Main product experiment C2 Fig. 17: Main impurity experiment C2

Table 11: Simulation results of experiment D2, distillation time is 5.8 hours

	Hold-up [Kmols]	x_1[methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.249	0.0000	0.0000	0.0070	0.9930
Vessel B	1.272	0.0000	0. 0335	0.9603	0.0062
Vessel C	2.582	0.0162	0.9666	0.0172	0.0000
Vessel D	0.897	0.9927	0.0073	0.0000	0.0000



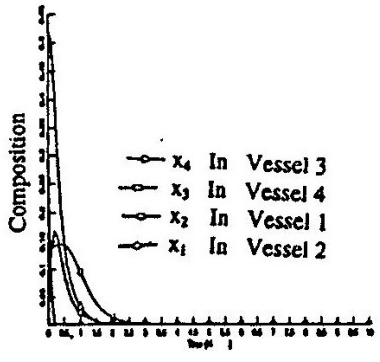
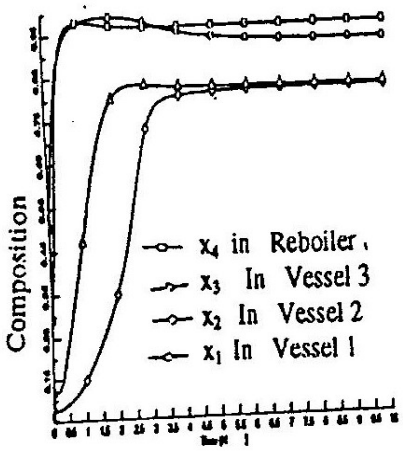


Fig. 18: Main product experiment D2 Fig. 19: Main impurity experiment D2

Table 12: Simulation results of experiment, distillation time is 7.0 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.276	0.0000	0.0000	0.0344	0.9655
Vessel B	1.013	0.0001	0.1100	0.8222	0.0677
Vessel C	2.924	0.0748	0.8164	0.1088	0.0001
Vessel D	0.786	0.9254	0.0745	0.0002	0.0000



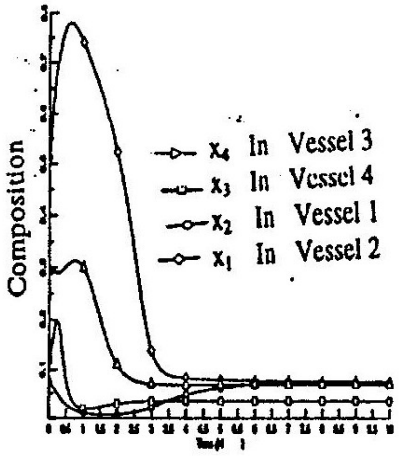
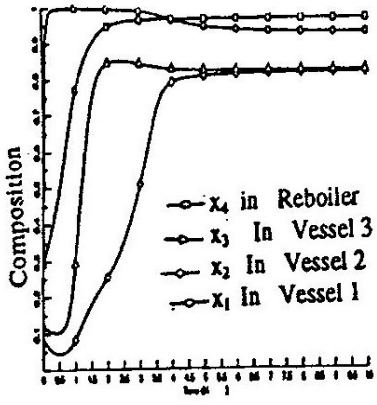


Fig.20: Main product experiment B3 Fig. 21: Main impurity experiment B3

Table 13: Simulation results of experiment B3, distillation time is 8.0 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.276	0.0000	0.0000	0.0344	0.9655
Vessel B	1.013	0.0001	0.1100	0.8222	0.0677
Vessel C	2.924	0.0748	0.8164	0.1088	0.0001
Vessel D	0.786	0.9254	0.0745	0.0002	0.0000



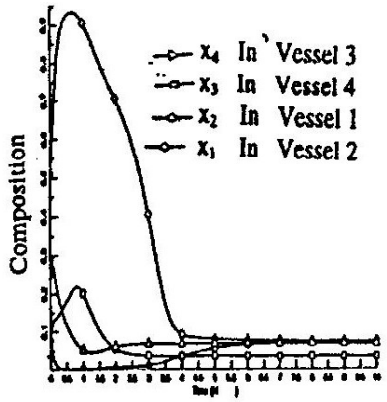
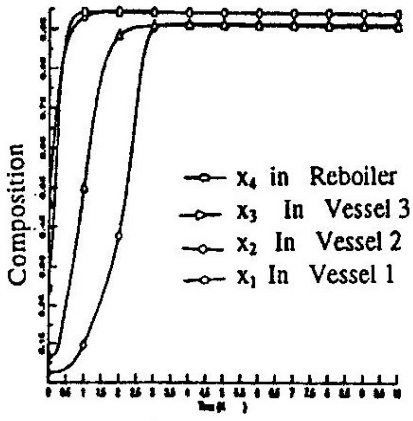


Fig. 22: Main product experiment B3 Fig. 23: Main impurity experiment B3

Table 14: Simulation results of experiment...., distillation time is 8.0 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.249	0.0000	0.0000	0.0070	0.9930
Vessel B	1.272	0.0000	0. 0335	0.9603	0.0062
Vessel C	2.582	0.0162	0.9666	0.0172	0.0000
Vessel D	0.897	0.9927	0.0073	0.0000	0.0000



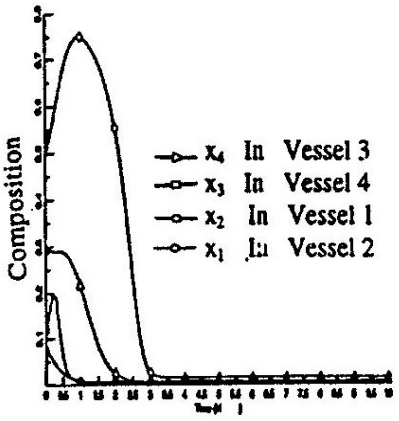
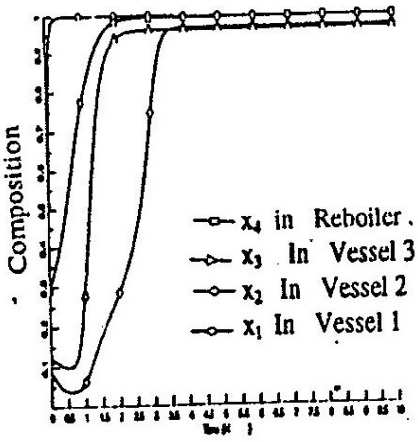


Fig. 24 Main product experiment C3 Fig. 25: Main impurity experiment C3

Table 15: Simulation results of experiment D3, distillation time is 5.5 hours

	Hold-up [Kmols]	x_1 [methanol]	x_2[ethanol]	x_3[n-propanol]	x_4[n-butanol]
Vessel A	5.249	0.0000	0.0000	0.0070	0.9930
Vessel B	1.272	0.0000	0. 0335	0.9603	0.0062
Vessel C	2.582	0.0162	0.9666	0.0172	0.0000
Vessel D	0.897	0.9927	0.0073	0.0000	0.0000



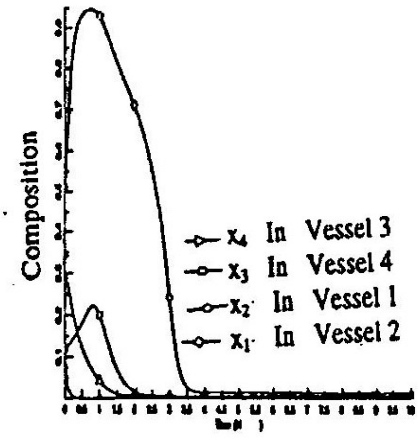


Fig. 26: Main product experiment D3 Fig. 27: Main impurity experiment D3

DISCUSSION AND CONCLUSION

In this paper a dynamic model of multivessel batch distillation column was developed and tested through simulation experiments. the simulation proved the feasibility of operation of multivessel batch distillation column as suggested by Hasebe et al (1995) and Skogestad et al (1995).

From the simulation results presented above, it has been observed that it is possible to separate multicomponent mixture into its purest form by using a multivessel batch distillation column. Also there is possibility of saving energy and time if compared to a regular multicomponent batch distillation column with same number of stages and efficiency(skogestad et al (1995)), which depends strongly on the reflux policy and use of off-cut to achieve the desired product composition.

Other observation are, by using control scheme utilizing temperature as suggested by Skogestad et al (1995), the final composition of the product at infinite time (steady state) does not depend on feed composition nor its redistribution in the vessels (see table of results and graphs), but increases with increased number of stages per section (see results of experimentA compared to C, and B as compared to D). Also through these results, if one look and compare the graph of experimentA to that of Experiment B, (as well as Experiment C and D), can detect the influence of initial hold-up in the vessel on start-up operation of the plant.

Though, the simulation results obtained are encouraging, more work is needed to be done. Further work planned to be done is:

* to develop a rigorous simulation model
* to build a pilot plant to verify the simulation results
* optimization study of the system
* determine limitation of operation for the system.

Also, it has been shown that the final composition of main product in the middle vessels are always lower than the final composition of the main product in the reboiler and upper vessel, which in other word is that the final composition of main product in the middle vessels can not be higher or equal to the composition of main product in the reboiler or upper vessel.

NOMENCLATURE

K	Number of stages
L	Liquid molar flowrate, $kmols^{-1}$
N	Number of components in the mixture
M	Molar hold-up, kmol
P	Number of column section
Q	Reboiler hear load, J/s
Q	Condenser heat load, J/s
TC	Temperature control
t	time, s
x	Liquid mole fraction
x	Feed mole fraction
V	Vapour molar flowrate, kmols
y	Vapour mole fraction
α	Relative volatility

Subscripts

b	Reboiler
c	Condenser
d	Distillate
i	Tray number
j,z	Component number
r	Reboiler
v	Vessel
w	Total number of stages

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