*Nigerian Research Journal of Chemical Sciences* **(ISSN: 2682-6054)**
**Volume 8, Issue 1, 2020**

# CONTROL OF A MULTICOMPONENT BATCH DISTILLATION PROCESS

Mahmud, H., Ochi, D.O., Aliu, S.O. and Ani, M.O.
Department of Chemical Engineering, Auchi Polytechnic, Auchi, Edo State, Nigeria
Corresponding Author: jabbal4luv@yahoo.com, lawekebafe@gmail.com

## ABSTRACT

The present study evaluated the comparative closed-loop performance of multicomponent non-reactive distillation followed by a much component reactive batch distillation column. The dynamic models of the non-reactive batch column was developed and simulated. Then three different control schemes, namely proportional integral (P1), Nonlinear proportional integral (NLPI) and gain scheduled proportional integral (GSPI), were designed. The control structures employed on the simulation experiments were conducted to examine the servo as well as regulatory performance. Then the dynamic simulation was performed to observe the column performance at start-up and production phase. The results showed that the time taken for the withdrawal of the lightest component is 91mins with purity of 0.985. The time for the intermediate component to reach the top of the column of 168m, was 77mins. GSPI controller strategy is thus recommended for a multicomponent batch distillate column compare to other two NLPI and P1 controllers because of the short time taken for distillation to be completed with high purity.

**Key words:** Batch process, control. Distillation multicomponent

## INTRODUCTION

The most widely used and oldest separation process used in unit operation by industries is the distillation process. This process has been around since 4000 BC. It was not until an Arabian alchemist name Jabir ibn Hayyan (721- 815 AD) invented the alembie shil that distillation became used for beverage purposes [1, 2]. Distillation process can separate two or more liquid components in a mixture using the principle of difference in volatility, the greater the non-linearity and the easier it is to separate the mixture using distillation. In the process, it involves the production of vapour by boiling the liquid mixture in a still and removal of the vapour from the shol by condensation. Because of differences in relative volatility or boiling points, the high component is rich in the liquid. In most cases, part of the condensate is returned back to the shol and is mixed

with the outgoing vapour. And this allows further transfer of higher components to the vapour phase and the liquid phase from the vapour phase. So the vapour stream becomes richer in light components and the liquid stream becomes richer in heavy components [3-5].

Literature has shown that several simulation experiments have been conducted on the multi-component batch distillation column in open and closed loop, but only few works have been done on the control of a batch distillation column. The relevance of this work is to obtain the column gain by calculation [5-7].

The batch distillation process is the oldest operation used for separation of liquid components for centuries and products of fine chemical and specialized products, such as alcoholic beverages, essential oils, perfume, manufacturing of pharmaceutical and petroleum products which is the frequent separation method in batch process [8, 9]

The aim of this work is to design a control system using the proportional integral denvation (PID) with the objective of obtaining a high pure distillate within a short time, using reflux ratio as the manipulating variable in controlling the amount of distillate obtained. It encompasses; an understanding of the modeling of batch distillation column.

## MODELING, SIMULATION AND CONTROL OF A MULTICOMPONENT BATCH DISTILLATION COLUMN

### PROCESS DESCRIPTION

In a batch distillation operation, two types of products are handled. The one named as slop-cut which is the byproduct of off specification material and the other named as product cut which is the product satisfying the specified purities. The operation of a batch column is divided into a number of repeated stages which includes the total reflux, withdrawal of the highest purified product, removal of a slop-cut, withdrawal of the highest purified product; removal of a second slop-cut and so on. If the aim of production is to separate each compound from the feed mixture at the specified purity levels, the number of product cuts is the number of compounds (NC) in the feed and the number of the maximum possible slop- cuts is NC-i Figure 1 shows the basic elements of a multicomponent batch distillation column (MBDC) system and their configuration. It consist of Reboiler, trays assembled in the column, coupled unit of condenser and reflux-drum, product and slop-cut storage tanks [10-12].

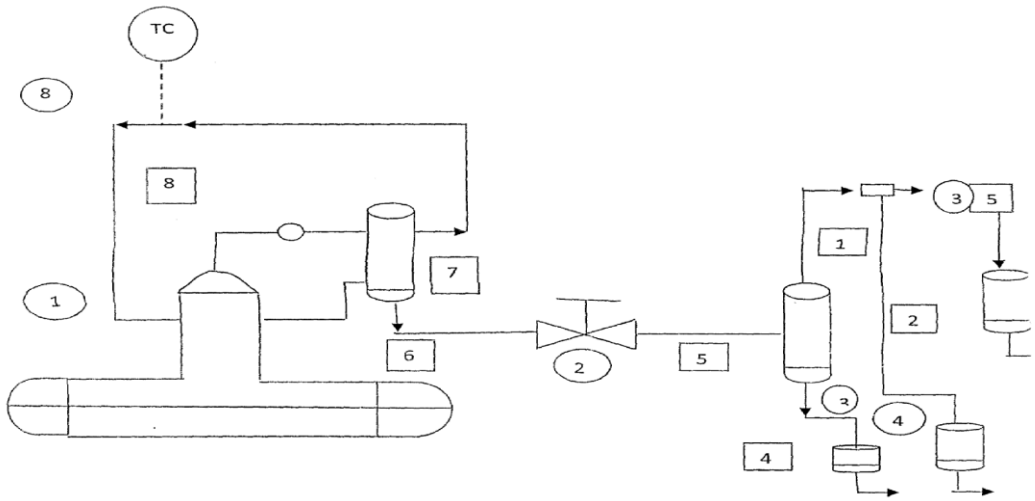



Figure 1: The process flow diagram using PRO 11

In order to represent realistic operation of actual batch distillation column a rigorous nonlinear model that considers simultaneous effect of heat mass transfer operations and fluid flow on the plate is needed. Such batch distillation model is derived from first principles involving dynamic material and component, and algebraic energy equations, support by vapour-liquid equilibrium and physical properties. The multicomponent batch distillation dynamics simulation has major computation functions like vapor flow, liquid flow and tray holdup calculations, enthalpy calculations, average molecular weight and density calculations, and vapour liquid equilibrium calculations [14,15].

The operation of batch distillation described here corresponds to a ternary system of cyclohexane toluene-chlorobenzene. Among these consistent feed components cyclohexane is the highest component; toluene is the intermediate component, and chlorobenzene is the heaviest component [16, 17].

**The model structure of the ternary distillation**

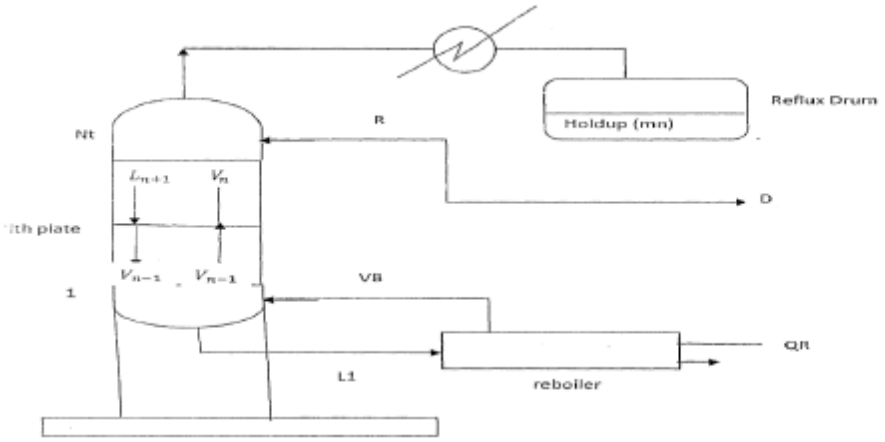



Figure 2: Schematic representations of the multicomponent batch distillation process

Process is developed based on the following assumptions:

1. Staged batch distillation column with trays numbered from the bottom and top (total 14 trays including still pot and reflux drum).
2. Perfect mixing and equilibrium on all trays.
3. Constant stage pressures (atmospheric and tray efficiencies (vapour — phase maximum efficiency 75%).
4. Negligible tray vapours holdups.
5. Total condensation with no sub cooling in the condenser.
6. Nonlinear francis weir formula (Luyben, 1990) for tray hydraulics calculations.
7. Variable liquid holdup in each tray.
8. Constant liquid holdup in the reflux drum (perfectly controlled by a conventional proportional (P) controller with proportional gain.
9. Raoult's law for the vapour liquid equilibrium.

Batch distillation is inherently an unsteady state process. Consider the distillation column as shown in Figure 2. Normally in batch processes the feed is charged in the still at the bottom of the column. For this study feed is a cyclohexane, toluene-chlorobenzene mixture, which has composition 0.4-0, 4-0.2 respectively. This mixture is to be separated by this batch process. The column shown in Figure 2, has 12 plates excluding reboiler and reflux drum. It was divided into five sections for

evaluation of the material and energy balances easily. MB is the amount of holding in the still. QR amount of heat s supplied to still [14-16].

Due to the heat feed in the still, the phase changes according to the relative volatility and VB amount of vapours were formed which tries to go up through the first plate and so on. On first plate there are four stream two inlet and outlets each. The suffix in the stream name showed the stream coming from that plate. For example $L_1$ is used for vapour rate. M for hold up, H for liquid enthalpy, V for vapour enthalpy, x is liquid composition and Y is vapour composition.

## MODELING EQUATIONS

Material balance, component balance and enthalpy balance equations were written accordingly. The change in the heat energy for a very small amount of time can be considered negligible i.e the change is very small.

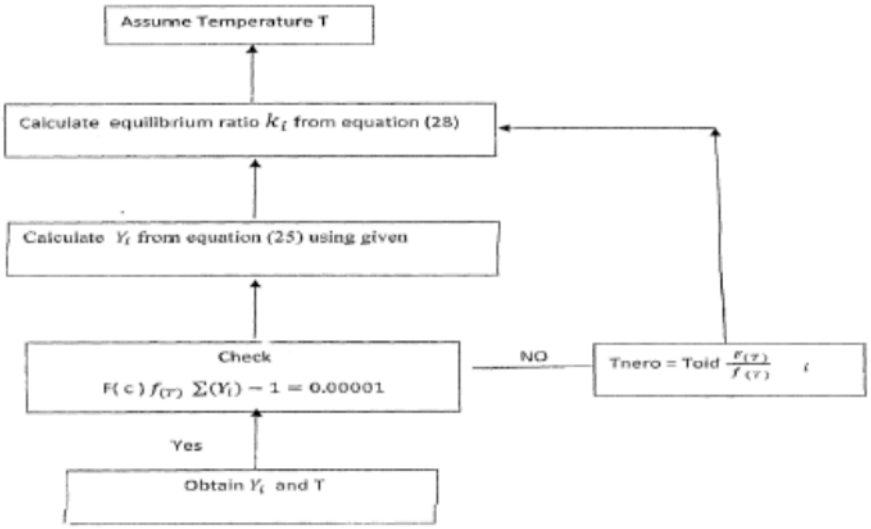



Figure 3: Calculation of temperature (t) and vapour composition

### Liquid Flow rate calculations

For the calculation of the liquid flow rate, the Francis weir, formula was used. Liquid flow rate is a function of density, molecular weight and tray parameters which include the tray holdup, height, length and column diameter. The change in the liquid rate is accounted for by changes in the density and indirectly the liquid composition [14, 18]

Density and molecular weight of liquid on the plate is calculated by the sum of product of liquid composition and density, and liquid composition and molecular weight of all the components present in the system respectively [19,20]

Table 1: Batch Distillation column specification

| | |
|---|---|
| System | Cyclohexane/toluene/chlorobenezene |
| Feed (Kmol) | 30 |
| Feed composition | 0.40/0.40/0.20 |
| Number of trays (Excluding Reboiler) | 12 |
| Tray hold-up (Kmol) | 0.03 |
| Heat input to still (kg/mm) | 25,00 |
| Distillation composition | 0.99 |
| Reflux drum hold-up (Kmol) | 1.0 |
| Production rate (Kmol/min) | 0.10 |
| Time step (min) | 0.005 |
| Column diameter (inch) | 18 |
| Weir length (inch) | 12 |
| Weir height (inch) | 0.30 |
| Murphee tray efficiency | 0.75 |

## CONTROLLER SYNTHESIS

In closed-loop simulation study, the control objective is to recover the light component and intermediate component at a constant purity. The manipulated input is the reflux flow rate. Distillate light component and intermediate components are controlled with any one of proportional integral (PT) controller. Nonlinear proportional integral (NLPI) controller and Gain scheduling proportional integral (GSPL) controller [21, 22].

### Nonlinear proportional integral controller

The idea of a non-linear proportional integral controller (NLPI) controller is to modify the controller action in some way to compensate for the nonlinearity to the process. This means that control output is effectively proportional to square of the error.

## CALCULATION OF GAIN (KC)

From a control point of view, a two product distillation column with a given feed have fine degrees of freedom (fine flow which can be adjusted L,V, Vr, D and B) at steady state. The assumption of constant pressure and perfect level control in the condenser and reboiler reduces the number of degrees of freedom to two. These two degrees of freedom can then be used to control the two

product composition, XD and XB (or some other indicator of composition, like the tray temperature).

## RESULTS AND DISCUSSION

Several simulation experiments have been carried out on the multicomponent batch distillation column in open loop as well as closed loop mode. The column is employed for the fractionation of hydrocarbon system. Cyclohexane-toluene-chlorobenzene is separated as distillate products and chlorobenzene is separated as a product in the still pot.

In batch distillation operation, first the column may be brought to the steady state by considering the total reflux startup procedure. Then the production phase is started and the controller switched on to maintain the specified product quality.

Sometimes the product is withdrawn as soon as the distillate composition reaches its desired value, without waiting for the steady state to be attained [3,23]. Notice that immediately after the production phase is started, controller responses may be very aggressive. It happens because of the following two reasons: (i) immediate withdrawal of the distillate product and (ii) the change of distillation.

### Composition from the steady state value to the set point value

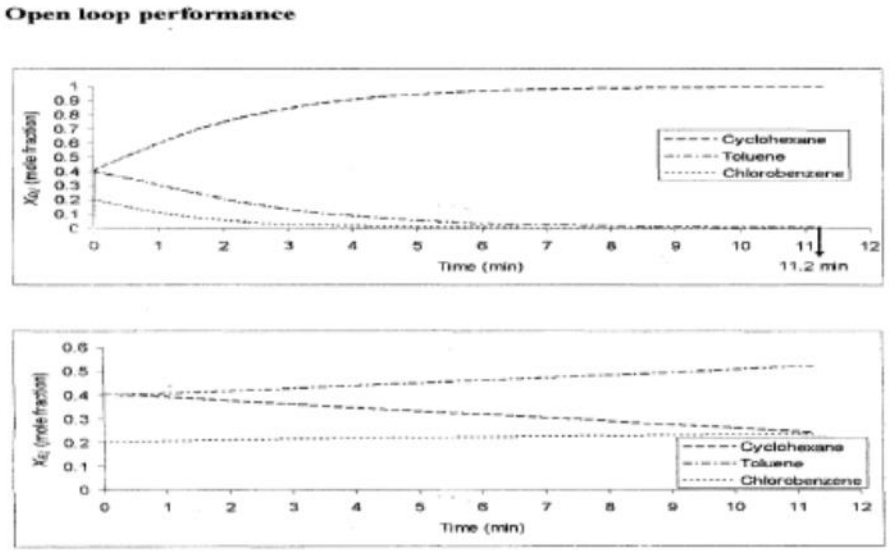



Figure 4: Open-loop process dynamics at start-up phase

Figure 4 presents the dynamics of the uncontrolled distillate composition of the example batch column at the startup phase. The steady state composition of the component column can be considered as a high purity distillation process.

Figure 5 illustrates the uncontrolled process dynamics at the production phase. The production phase has been started from the steady state arid with the withdrawal of distillate,

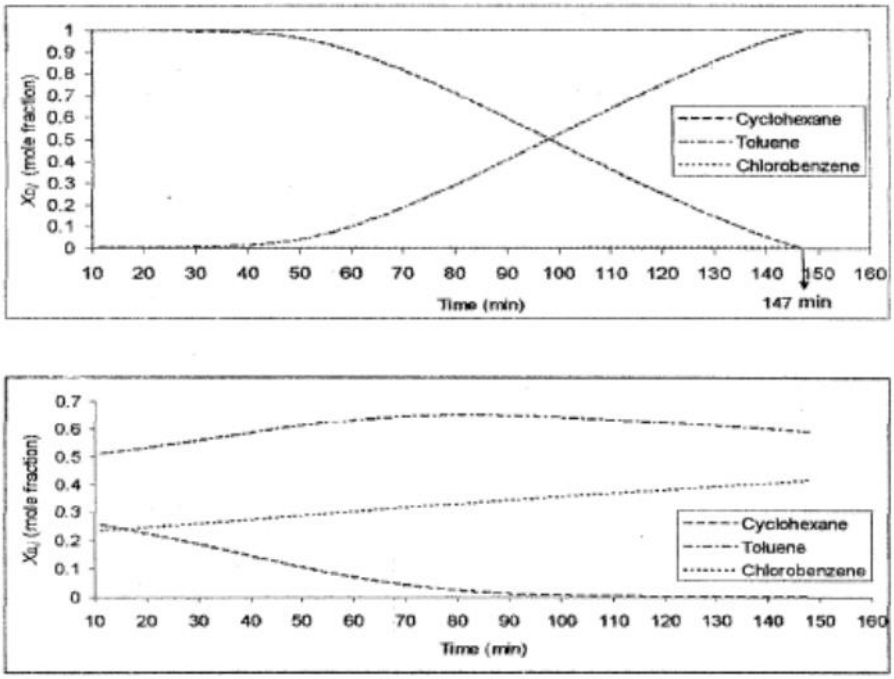



Figure 5: Open-loop process dynamics at the production phase

## CONSTANT COMPOSITION CONROL

In the present study, the set point composition has been fixed at a value of 0.985 for lightest and 0.97 for intermediate component. The column is started up as usual and the lightest component withdrawal is begun as soon as this component met the composition specification, then set point step change is maintained from 0.995w 0.985 at time 30 min. The constant composition control is continued until the distillate decrease to small almost zero value. The time taken to the withdrawal of the lightest component is 91 min with purity of 0.985. At this moment the controller is switched off and the intermediate component starts to reach the top of the column, time period 77 min. Then this component has reached the desired purity (XDSP 2 0.97), constant composition control is started again. In between the withdrawal of the lightest and intermediate components, the distillate

is collected at the slop cut. At this moment we must note that in the simulation experiment, the distillate flow rate is, manipulated by a proportional level controller to maintain constant (rarely) liquid holdup in the reflux accumulation. The time taken to withdrawal the second highest component is 66mins with purity 0.97. At this moment the controller is switched off during the second slop cut, third component starts to reach the bottom of the column up to purity of 0.938 [9,18].

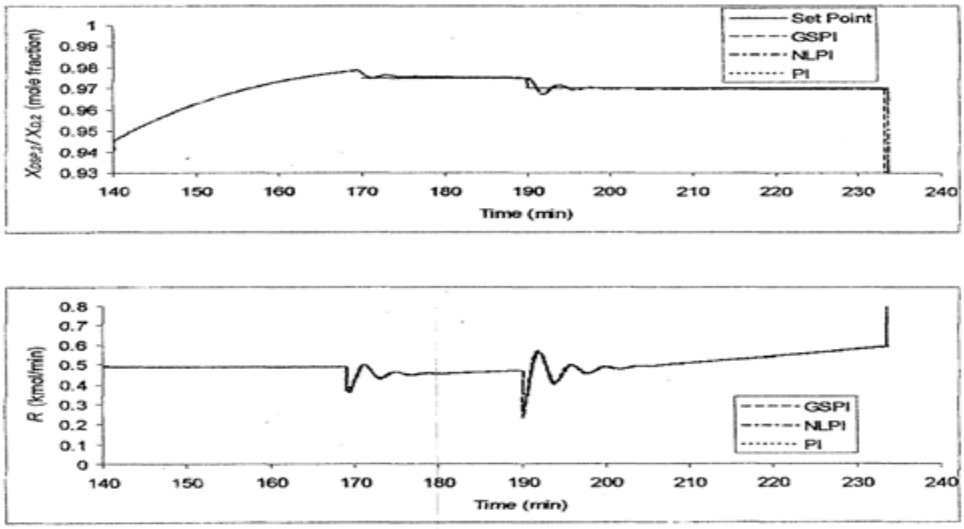



Fig.5b.Comparative closed loop performance of PI, NLPI and GSPI control algorithms with a set point change in $X_{D,2}$ (0.975 to 0.97 at time=190 min)

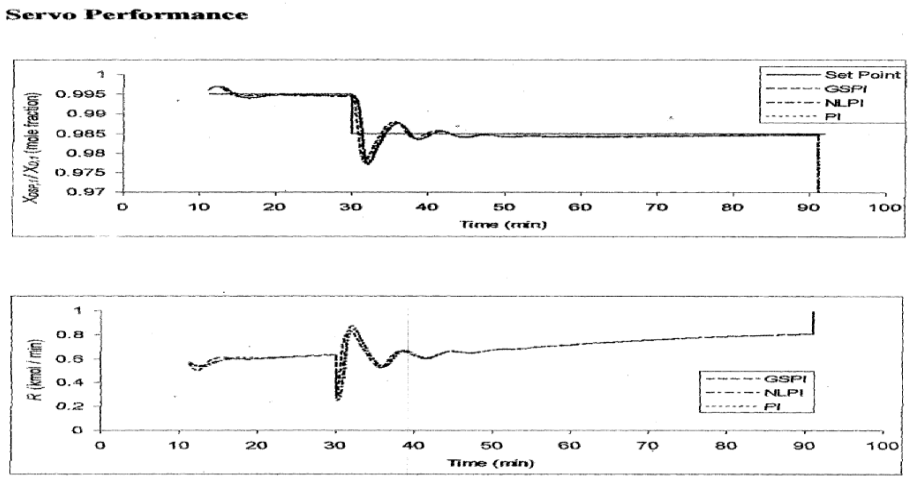



**Fig.5a. Comparative closed loop performance of PI, NLPI and GSPI control algorithms with a set point change in $X_{D,1}$ (0.995 to 0.985 at time=30 min)**

Withdrawal of highest and intermediate components are shown in Figure 5a and 5b with servo performance (+5% step change inset point) at time 30 min and 190 min.

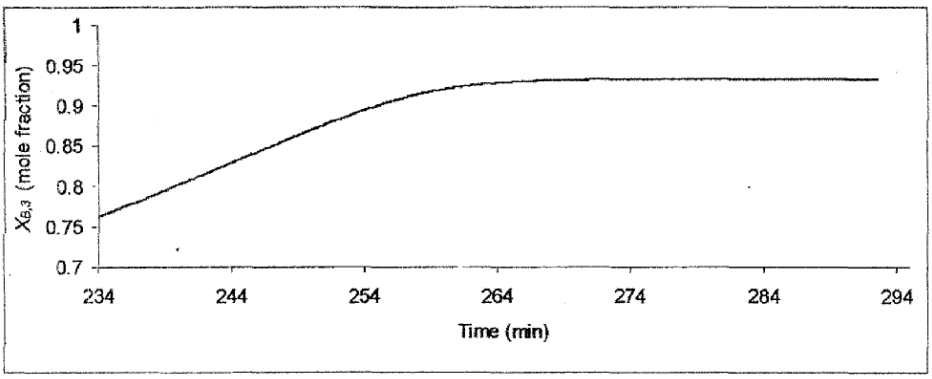
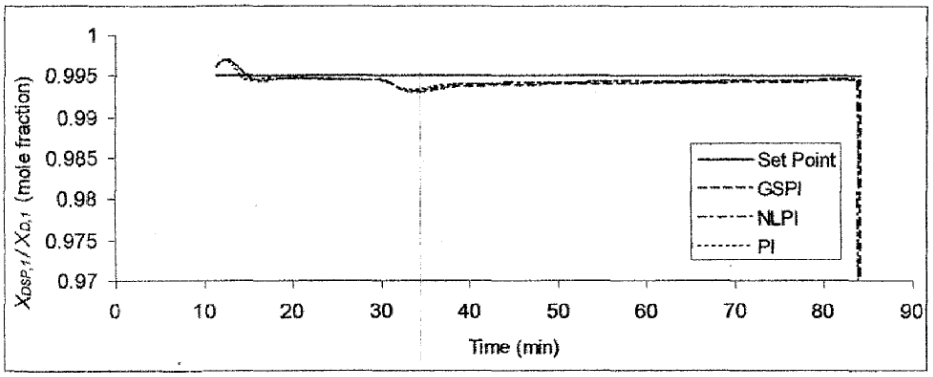



Fig.5c.Third component in the bottom after second slop cut

**Regulatory performance**



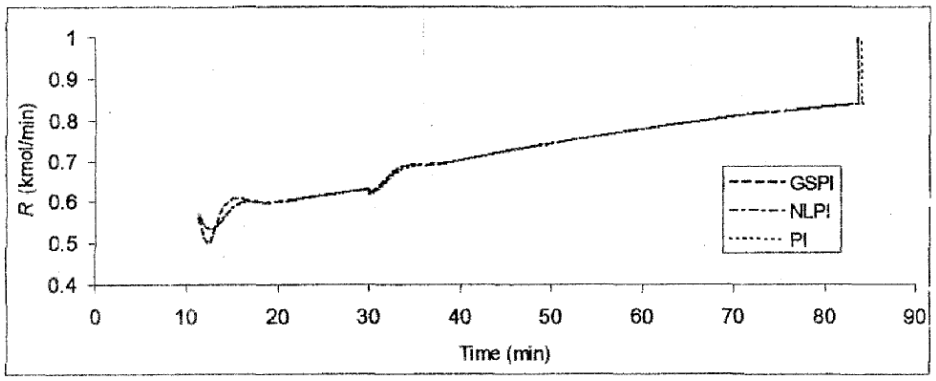




Fig.6a.Comparative Regulatory performance of PI, NLPI and GSPI control algorithms with +5% (25000 ⟶ 26250 kJ/min ) step change in reboiler heat duty at time =30min.

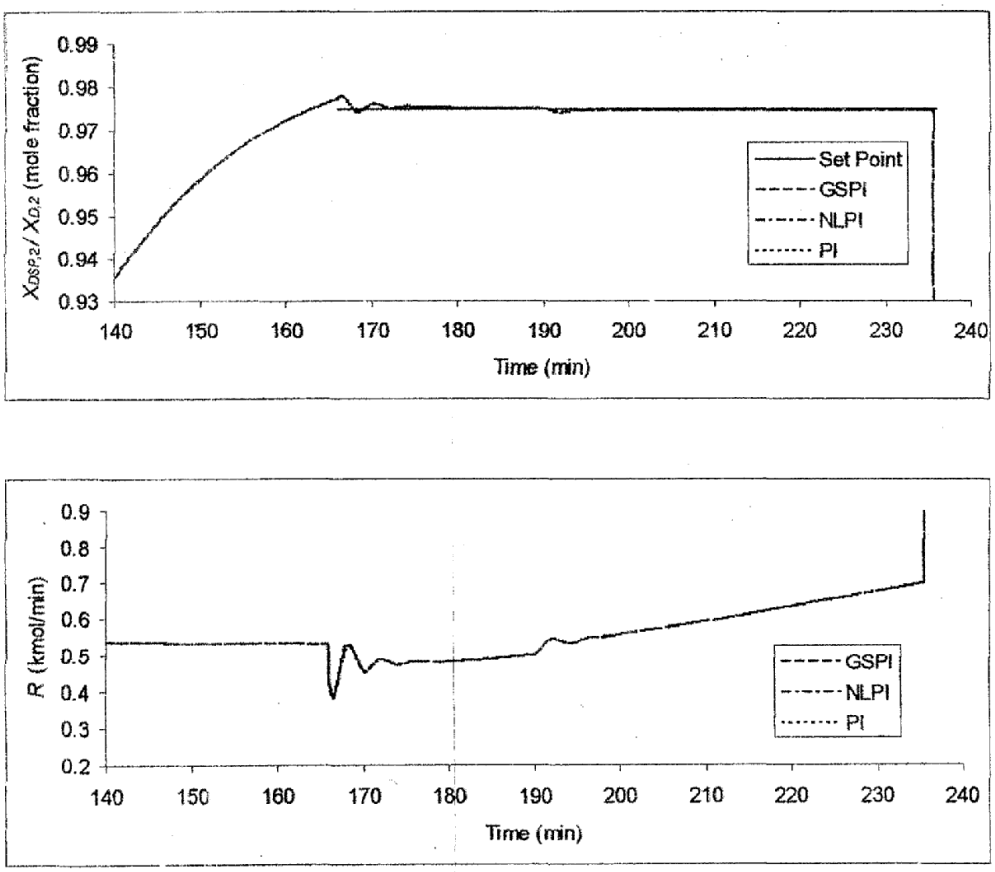



Fig.6b.Comparative Regulatory performance of PI, NLPI and GSPI control algorithms with +5% (26250 ⟶ 27562 kJ/min ) step change in reboiler heat duty at time =190 min.

Table 2: Regulatory performance for $X_B$ change for component $X_{D,1}$

| Controller | *Kci* | $\tau_i$ | *a* | ISE |
|---|---|---|---|---|
| PI | 35.65 | 6.5 | ---- | 0.000019565 |
| NLPI | 35.65 | 6.5 | 12.5 | 0.000019283 |
| GSPI | 35.65 | 6.5 | ---- | 0.0000152386 |

Liquid level in the reflux drum controlled by proportional controller. Tuning parameter for proportional controller *kcm*= -0.0005

Table 3: Regulatory performance for $X_B$ change for component $X_{D,2}$

| Controller | *Kci* | $\tau_i$ | *a* | ISE |
|---|---|---|---|---|
| PI | 38.68 | 7.5 | ---- | 0.000058637 |
| NLPI | 38.68 | 7.5 | 12.1 | 0.000055245 |
| GSPI | 38.68 | 7.5 | ---- | 0.000043618 |

Liquid level in the reflux drum controlled by proportional controller. Tuning parameter for proportional controller *kcm*= -0.00052

## CONCLUSION

The comparative closed-loop performance of multicomponent non-reactive distillation followed by a much component reactive batch distillation column has been evaluated using the multicomponents control system. The control structures were employed on the simulation experiments conducted to examine the servo as well as regulatory performance. Then the dynamic simulation was performed to observe the column performance at start-up and production phase. Therefore the GSPI controller strategy is proposed for a multicomponent batch distillate column compare to other two NLPI and P1 controllers.

**REFERENCES**

[1] Barolo, M., Berto, F. (1998) Composition control in batch distillation Binary and Multicomponent mixtures. *Industrial and Engineering Chemistry Research* 37 (12), 4689-4698

[2] Luyben, W. C, (1990). Process modeling, simulation and control for chemical Engineers. Mc Graw-Hill, 2nd edn, Singapore, 72-74, 133-138 and 157 — 162.

[3] Almila, B. & Canan, 0. (2008). State estimation for a reactive batch distillation column. Proceedings of the international federation of automatic control, pages 1 — 6.

[4] Swapna Reddy P., Sachin C. Patwardhan, K. Yamuna Rani (2019). Robust Trajectory Tracking in a Reactive Batch Distillation Process using Multirate Nonlinear Internal Model Control. *Industrial & Engineering Chemistry Research*, 58 (26) 11364-11381.

[5] Bonsfills, L. Puigjaner (2004). Batch distillation: simulation of multicomponent Batch rectification with chemical reaction. *Computer Chemical Engineering* 10, 389 - 398.

[6] Albert, J. M., Ic lann, J. M., Joulia, X. & Rcehret, B. (1991). Rigorous simulation of Multi-component multisequence batch reactor distillation, *Computer- Oriented Process Engineering*, 75, 75-80.

[7] Amiya K. Jana (2007). Synthesis of nonlinear adaptive controller for a batch distillation, *ISA Transactions*, 46, 49 — 57

[8] Bequette, B, W. (2006). Process control: modelling Design and simulation, Prentice — Hall, mc, New Delhi, 359- 362.

[9] Henley, E., Seader, J. (1981). Equilibrium stage separation operation in chemical Engineering John Wiley and Sons, Inc., 2nd edn, New York, 714 — 724.

[10] Jana, A. K., Samanta, A. N., & Ganguly, S. (2005). Globally linearized control system design of a constrained multivariable distillation column; *Journal of process control* 15,169—181.

[11] Mujtaba, I. M., Macchietto, S. (1997). Efficient optimization of batch distillation with Chemical reaction using Polynomial curve fitting techniques, *Industrial Engineering Chemical Research* 36, 2287- 2295.

[12] Warter, M., Demicoli, D., & Stichimair, J. (2004). Operation of a batch distillation column with a middle vessel: Experimental results for the separation of zeotropic and azeotropic mixture, Chemical Engineering and Processing: Process Intensification, 43 (3), 263-272.

[13] Maryaret. J Eppstein & David E. Dougherty (1996). Simultaneous estimation of transmissivity values and zonation. *Water Resources Research*, 32 (11), 3321-3336

[14] Moshood, J.0., Al-Arfaj, M. A. (2006). Estimator — based control of reactive distillation system: Application of an extended K, *Chemical Engineering Science*, 61(10), 3386-3399

[15] Kanagaraj, N., Sivashanmugam, P. & Paramasivam, S. (2009). A fuzzy logic based supervisory hierarchical control scheme for real time pressure control, *International Journal of Automation and Computin*g, 6, 88-96.

[16] Stathis Skouras and Siguard Skogestad Analysis and control of heteroazeotropic batch distillation, *AIChE Journal* 51 (2005) 1144–1157

[7] Sorensen, E. & Skogestal, S. (1994). Optimal state estimation of multicomponent batch Distillation, *Chemical Engineering Science*, 56, 5771 — 5786.

[18] Geir. E, (1992). Using the extended filler with a multi-layer Quasi-Geostrphic octarrnodel, *RNAL of Geo-physical resource*, 97, 1 — 17.

[19] Modla, G. P. Lang, P. (2008) Feasibility of new pressure swing batch distillation methods, *Chemical Engineering Science*. 63 (2008) 2856–2874

[22] Denes, F., Láng, P., & Joulia, X. (2009). Heteroazeotropic batch distillation in a new double-column system. In *Chemical Engineering Transactions* 18, 713-718).

[21] Eliana Zamprognaa , Massimiliano Baroloa, Dale E. Seborg (2004) Estimating product composition profiles in batch distillation via partial least squares regression. *Control Engineering Practice* 12, 917–929

[22] Arpad K, Gabor, M and Pete L, (2009) Operation and control of a new pressure swing batch distillation system. *Chemical Engineering Transactions*, 18, 1- 6

[23] Galindez, H., fredenslund, A A, (1988) Simulation of multicomponent batch distillation Processes. *Computers and Chemical Engineering*, 12, 281 — 288