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Model and simulation of a distillation column applied to the propylene / propane mixture

[1]Milton Jiménez, [2]Olga Ramos, [3]Darío Amaya

[1]Research Assistant, Mechatronic Engineering, Nueva Granada Military University, Bogotá, Cundinamarca, Colombia.
[2]Professor and Research, Mechatronic Engineering, Nueva Granada Military University, Bogotá, Cundinamarca, Colombia

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Address For Correspondence:
Milton Jiménez, Nueva Granada Military University, Mechatronic Engineering, Faculty of Engineering, 57+16500000 – Ext 1280, Bogotá Colombia.

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BACKGROUND
The separation of mixtures is in particular one of the processes in which more energy is used in the petroleum industry, since it is usually carried out by distillation at high temperatures.

OBJECTIVE
Model and simulate a process of distillation of the compound from a hydrogenation system of propyne and propadiene, for the production of polymer grade propylene and propane to be delivered to the gas network

RESULTS
The dynamic model was evaluated evidencing the behaviour of the fractionation column with his profiles of the temperature, compositions of the mixture, due to the slow dynamics of the process it was necessary to use 2 $x10^4$ samples for obtaining trends of the compositions in the head and the bottom of the column.

CONCLUSION
The type of distillation presented shows advantages, due to the high efficiency that allows obtaining for a maximum performance, directly impacting the operating costs allowing their reduction, on the other hand, this type of columns was easy to use taking into account only it was necessary to maintain the conditions of operation, which were easy to follow.

KEY WORDS
Modelling system, distillation, olefins plant

INTRODUCTION

The olefins in which are used with propylene/propane are important chemical precursors used in industrial processes [1]. Low temperature distillation technology is commonly used to obtain high purity compounds [2]. Allowing their use in different areas, such as laboratory equipment, automotive sector, textiles among others [3].

The development of processes for obtaining and separating propylene / propane, are becoming of great importance in the world, given his economic viability. However, these processes are highly complex, given the physicochemical characteristics presented at the molecular level [4]. In search of a greater productivity in this type of process, it was necessary to develop a type of column that would perform the distillation at low temperatures with lower energy consumption, there is when arise the HIDiC (*Heat-Integrated Distillation Column*) [5], [6].

This type of columns presents a greater energy efficiency than others, due to the advantage of the proximity between the boiling points of the components to be separated, allowing to reduce the number of heat exchangers, allowing an energy saving of up to 60% [7].Taking into account the number of stages that constituting it traditionally, the energy saving is seen between two or three times with respect to a conventional column [8]. In addition it can operate at a lower compression ratio, relative to the heat source [9].

In [10], a simulation was proposed that allows the analysis of the modelling of the column in combination with hybrid membranes (HMD), in order to increase the purity of the product obtained, in ethylene it was evident that for the serial system it was more Economic, but when his configuration was in cascade increases more his purity.

In [11], it presents the dynamic simulation of a HIDiC column, based on the equilibrium models. It develops a simulator for dynamic distillation columns by analysing the rectification section, the behaviour in his vapor phase and the dynamic energy balance, taking into account the state equation (SRK) used in hydraulic systems.

In [12], the simulation of the HIDiC column shows the heat transfer performance, finding practical applications in which it could save up to 30% of energy, compared to conventional distillation..

Based on the above, in this paper, the results were presented after modelling and simulating a process of distillation of the compound from a hydrogenation system of propyne and propadiene, for the production of polymer grade propylene and propane to be delivered to the gas network

METHODS AND MATERIALS

In the process of distillation, the different compounds to be separated are store in a tank or column. The process starts when heat or caloric energy is introducing into the bottom of the tank. The energy is introduce into the bottom by a heater, in order to generate the vapor that will constitute an upward flow in the column [13]. The column inside has a distribution of overflows which are known as "plates". In each of them, simpler distillations of each of the components in the mixture are performed, combining the liquid and gaseous phases that go in opposite directions. Allowing the generation of a balance between the energies of the liquid phases and the gaseous phases [2].

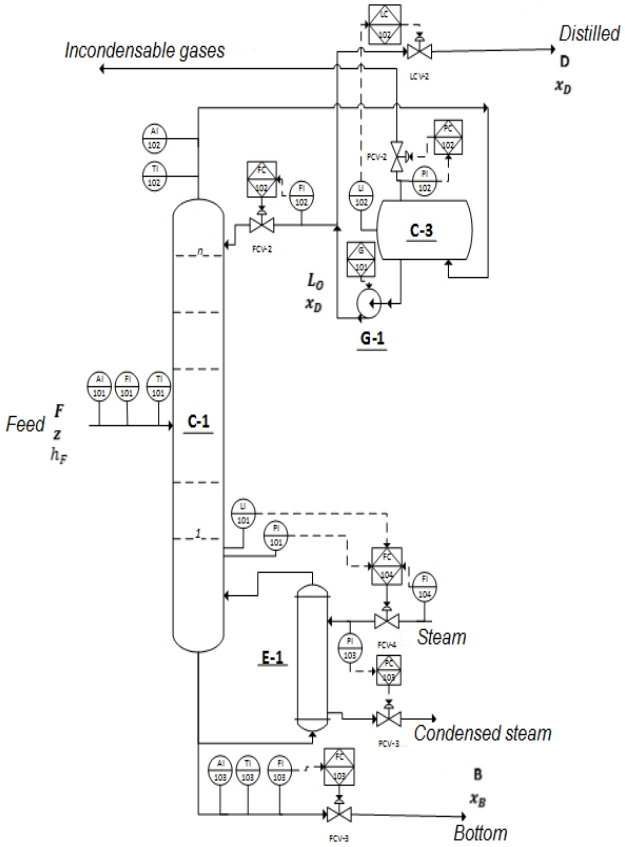

Fig. 1: Diagram of the column

The Fig. **1** shows the diagram of a distillation column with a total condenser and a thermosyphon heater, in which they were shown the feed rates, the output head, the bottom and the flows which are respectively shown: F, D, B y L_0. Also, the compositions of the products over time and the molar fraction of the feed components were also shown x_D, x_B, z y b. Given the input enthalpy flow: h_F.

The product flows depend on the conditions in the plates, the heater and the condenser, which causes the division of the column in a certain amount of volumes, one for each plate, besides those corresponding to the condenser and the heater [9]. For each of these volumes, the N material balances and the N energy balance equations (enthalpy) must appear, where N was the number of components, which for this particular case were two (propylene and propane) [14].

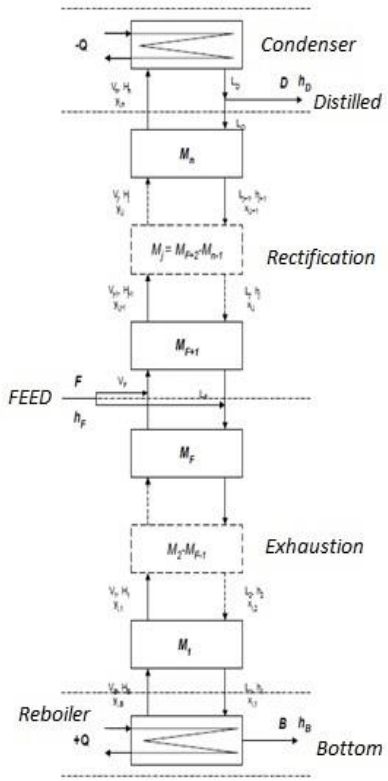

Fig. 2: Diagram of the column

In Figure 2 shows the block diagram of the system. Where mass and energy fluxes (enthalpies) were observed, showing the different stages in which the distillation process was carried out: exhaustion and rectification, as well as the phases of the matter and energy balance equations: feed, reflux, condenser and heater

Plate-column equations C-1. The equations of the plate were those that allow to describe the balances of a plate, contemplating the zone of exhaustion and rectification.

Starting from the previous one it was necessary to perform the analysis of the plates of the column in each of the sections, for this, it was taken as a basis the scheme of the plate shown below:

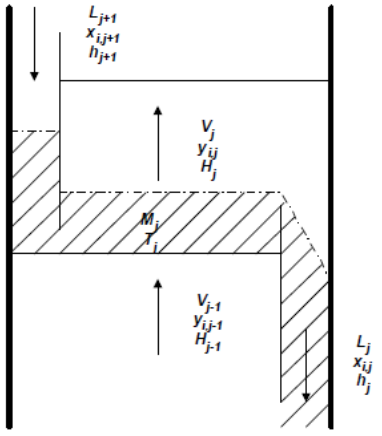

Fig. 3: Schematic of the plate column.

Source: *Modelling and neuro control for multicomponent nonideal distillation column* [15]

The total mass balance when there weren't chemical reactions, can be expressed in molar units, considering a low density, the mass accumulation of the vapor phase in relation to the liquid phase was negligible, whereby the equation of the total mass balance in plate j would be given by [16]:

$$\frac{d}{dt} M_{lj}(t) = L_{lj+1}(t) + V_{lj-1}(t) - V_{lj}(t) \quad (1)$$

Where:
$M_{lj}(t)$– Residual liquid in the plate *lj* [mol].
L_{lj} – Flow of exit liquid of the plate *lj* [mol/s].
$V_{lj}(t)$ – Flow of exit steam of the plate *lj* [mol/s].
$L_{lj+1}(t)$ – Liquid flow from the upper plate [mol/s].
$V_{j-1}(t)$ – Steam flow from the lower plate [mol/s].

It is necessary to contemplate that the liquid in the plate was perfectly mixed, so that the properties of the liquid leaving the plate were equal to those of the liquid that remains in it [17]. Without this approach, it would be necessary to represent the balances for each of the plates, through partial differential equations, increasing the level of difficulty of the problem. Thus, equation (2), represents the balance of component *i* in the plate *j* [18]:

$$\frac{d}{dt}\left(M_{lj}(t) \cdot x_{e,lj}(t)\right) = L_{lj+1}(t) \cdot x_{e,lj+1}(t) + V_{lj-1}(t) \cdot y(t) - L_{lj}(t) \cdot x_{e,lj}(t) - V_{lj}(t) \cdot y_{e,lj}(t) \quad (2)$$

Where:
$x_{e,lj}(t)$ – Mole fraction of the compound *e* of the exit liquid from the plate *lj*.
$y_{e,lj}(t)$ – Mole fraction of the compound *e* of the exit steam from the plate *lj*.

Equation 2 was applied to the N-1 components in each plate dish, taking into account that the sum total of the molar fractions must be equal to 1.

$$\sum_{i=1}^{N} x_{i,j}(t) = 1 \quad (3)$$

The number of variables per plate will be (2N + 3), particularly for this case were seven (7):

- Four (4) to describe the compositions of propylene and propane in two phases.
- Two (2) for flow rates leaving the remaining phases and the moles of liquid that remains as residue on the plate.
- The balance of the different energies at each plate of the column.

$$\frac{d}{dt}\left(M_{lj}(t) \cdot h_{lj}(t)\right) = L_{lj+1}(t) \cdot H_{lj+1}(t) + V_{lj-1}(t) \cdot H_{lj-1}(t) - L_{lj}(t) \cdot h_{lj}(t) - V_{lj}(t) \cdot H_{lj}(t) \quad (4)$$

Where;
$h_{lj}(t)$ - Enthalpy of the liquid on the plate *lj* [J/mol].
$h_{lj+1}(t)$ - Enthalpy of liquid from the upper plate [J/mol].
$H_{lj}(t)$ - Enthalpy of the exit steam in the plate *ij* [J/mol].
$H_{lj+1}(t)$ - Enthaply of the steam from the bottom plate [J/mol].

At this point, there were two new variables, which correspond to enthalpies, one from the liquid state *(hlj(t))* and the other from the vapor state *Hlj(t)*), these two enthalpies were obtained from the plate.

In order to calculate the new variables, it was necessary to work with thermodynamics as well as to use other relationships. The composition of the steam can be obtained from the relation of Murphree for the efficiency of a plate [19], This value was assumed constant for all dishes of the column:

$$\eta_{M=\frac{y_{e,lj}(t)-y_{e,lj-1}(t)}{\dot{y}_{e,lj}(t)-y_{e,lj-1}(t)}} \quad (5)$$

Where
η_M -Efficiency for the plate according to Murphree, it was defined as 0.7.
$Y_{e,lj}(t)$ -Molar fraction of the compound and in the vapor in equilibrium with the liquid leaving the plate *lj*.

Applying equation 5 to each component present in each of the plates two additional equations were obtained, in these were added two variables corresponding to the equilibrium molar fractions [20].

$$\dot{y}_{e,lj}(t) = K_{e,lj}(t) \cdot x_{elj}(t) \quad (6)$$

Where

$K_{e,lj}(t)$ - Equilibrium coefficient for the compound *e* in the plate *lj*.

In order to find the value of the equilibrium coefficient, which was related to the variables of the pressure and temperature that was given in each one of the different plates and the values that were given from the nomogram of Scheibel and Jenny [21].

Starting from the fluid dynamics, it can be obtained a representation of the relation between the moles of the liquid that remain in the plate and the flow that comes out of it. Using the Francis equation [22], we obtain:

$$L_{lj}(t) = k \cdot \rho_{lj}(t) \left(\frac{M_{lj}(t) - M_{0,lj}(t)}{AT \cdot \rho_{lj}(t)}\right)^{\frac{3}{2}} \quad (7)$$

$\rho_{lj}(t)$ - Density of the liquid [mol/m^3].
$M_{0,lj}(t)$ - Retained liquid in the plate *lj* [mol].
AT - Cross area [m^2] for the plate.
k - Coefficient of landfill [m$^{3/2}$/s].

Replacing, it was obtained [15]

$$M_{0,lj}(t) = v \cdot \rho_{lj}(t) \quad (8)$$

Where *v* corresponds to the volume capacity contained in the plate when there was no flow in m^3.

Inside the system different enthalpies were experienced, the compounds were in the liquid and gaseous state, flowing through the plates, in order to be able to determine this variable one must take into account the different temperatures, with the peculiarity that for the liquid state the relation between Temperature and the existing heat capacity can be considered linear. In this process, the maximum difference of the head plate with the bottom plate, which was 4 K [6]

With the above, we proceed to determine the enthalpy based on the caloric capacity of each of the components [23].

$$h_{lj} = x_{e,lj} \int_{T_0}^{T_f} C_{pl} \cdot dT \quad (9)$$

Obtaining the next expression:

$$h_{lj}(t) = h(T_{lj}(t)) \quad (10)$$

In the same way, the enthalpy of the substances in the gaseous state was determined as a function of the temperature of each of the plates.

$$H_{lj} = y_{e,lj} \int_{0}^{T_f} C_{pv} \cdot dT \quad (11)$$

Based on the variation of the density of hydrocarbons in the liquid state [24], it can be considered for the temperature/density ratio in small temperature ranges, these liquids were incompressible allowing to establish a linear relation that can be described from the following form [25].

Equations for the feed plate, the C-1 column:

The plate on which the system power was performed was called *lj*. it was added to the previously determined representation where the flow, the enthalpy of the liquid and the fraction of the input component were found [26].

$$\frac{d}{dt}\left(M_{lj}(t) \cdot x_{e,lj}(t)\right) = L_{lj+1}(t) \cdot x_{e,lj+1}(t) + V_{lj-1}(t) \cdot y(t) - L_{lj}(t) \cdot x_{e,lj}(t) - V_{lj}(t) \cdot y_{e,lj}(t) + L_g(t) \cdot x_{eG}(t) \quad (12)$$

$$\frac{d}{dt}\left(M_{lj}\,(t)\cdot h_{lj}(t)\right) = L_{lj+1}(t)\cdot H_{lj+1}(t) + V_{lj-1}(t)\cdot H_{lj-1}(t) - L_{lj}(t)\cdot h_{lj}(t) - V_{lj}(t)\cdot H_{lj}(t) + L_g(t)\cdot h_g(t) \quad (13)$$

$L_g(t)$ - Feed flow [mol].
$x_{e,G}(t)$ - Mole fraction of the compound e in the feed liquid.
$h_G(t)$ - Enthalpy of feed liquid [*J/mol*].

Equation of the lower plate of C-1. For the first plate in the lower part, intervene the respective variables that were in the operations carried out in the bottom of the column, given the above, the equations for this plate [15], must be modified, obtaining the following:

$$\frac{d}{dt}\,(M_A\,(t)\cdot x_{A,lj}(t)) = L_B(t)\cdot x_{A,B}(t) + V_{S1}(t)\cdot y_{e,SA}(t) - L_A(t)\cdot x_{e,A}(t) - V_A(t)\cdot y_{e,A}(t) \quad (14)$$

$$\frac{d}{dt}\,(M_A(t)\cdot h_A(t)) = L_B(t)\cdot h_B(t) + V_{SA}(t)\cdot H_{,SA}(t) - L_A(t)\cdot h_A(t) - V_A(t)\cdot H_A(t) \quad (15)$$

$y_{lj,SA}\,(t)$ - Mole fraction of compound e in inlet steam stream in the plate A.
$V_{SA}(t)$ - Feed flow of steam for the plate A, [mol/s].
$H_{SA}(t)$ - Enthalpy of the steam inlet in plate A [J/mol].

Equation plate of the header:

For this plate, the equations previously worked in other plates were combine, it should be considered flow exception for the reflux liquid.

The equations of matter and energy balance will be given by [12]:

$$\frac{d}{dt}\,(M_{lj}\,(t)\cdot x_{e,lj}(t)) = L_{OA}\cdot x_{e,OA}(t) + V_{lj-1}(t)\cdot y_{e,lj-1}(t) - L_{lj}(t)\cdot x_{e,lj}(t) - V_{lj}(t)\cdot y_{e,lj}(t) \quad (16)$$

$$\frac{d}{dt}\left(M_{lj}\,(t)\cdot h_{lj}(t)\right) = L_{OA}\cdot h_{OA}(t) + V_{lj-1}(t)\cdot H_{lj-1}(t) - L_{lj}(t)\cdot h_{lj}(t) - V_{lj}(t)\cdot H_{lj}(t) \quad (17)$$

L_{OA} - Flow rate [mol/s].
$x_{e,OA}(t)$ - Molar ratio of compound *e* in the liquid flow.
$h_{OA}(t)$ - Molar enthalpy of liquid [*J/mol*].

Results analysis:

The mathematical model obtained, allows the representation of the industrial process. The developed model describes the dynamic behaviour by means of continuous variables analogies in time.

After this, the validation of the models was done by the simulation of each one of them, for this the Matlab 2013[a] software was used, the dynamic model was evaluated evidencing the behaviour of the fractionation column with his profiles of the temperature, compositions of the mixture. Due to the slow dynamics of the process it was necessary to use 2 x10^4 samples for obtaining trends of the compositions in the head and the bottom of the column, as shown in Figure 4 below.

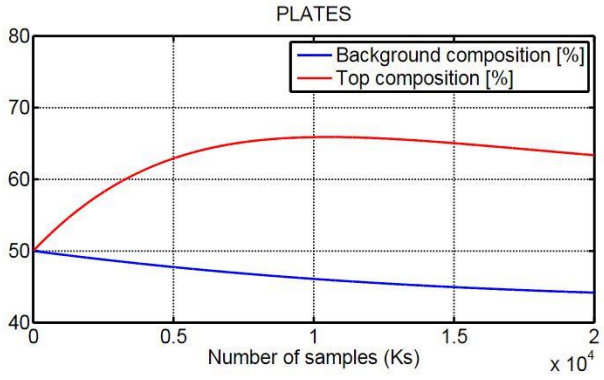

Fig. 4: Bottom and head compositions

It was obtained profiles on composition and temperature for each of the plates of the column as shown in Figure 5.

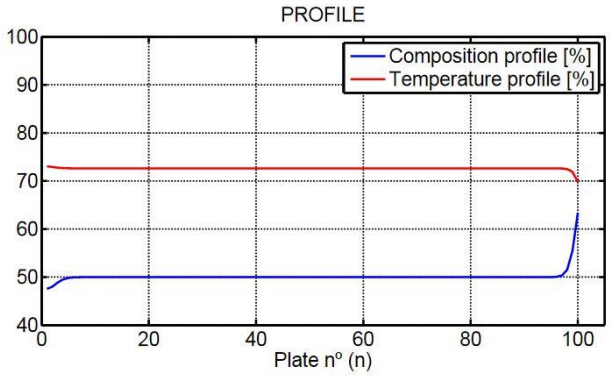

Fig. 5: Temperature profiles on plates.

The profile of compositions shown in figure 5 shows the behaviour in the sections of the column, in the section of rectification it presented an increase in the composition up where the rectification begins, in this section given the ascending and descending flows of the components in each of his phases presents a stable behaviour remaining at 50%. For last section in which the condensation occurs, the gaseous component counts with a higher percentage and then passes to the condenser.

The temperature profile shown in figure 5 shows the delta temperature with which the column counts, it corresponded to 4 K having the maximum heat transfer between plates number 5 and 95.

Conclusions:

The number of design variables for the distillation column give his complexity, this was determined by the sum of the variables of the compounds to be processed, contemplating the restrictions that can present the compositions.

The restrictions contemplate the currents that exist in each one of the elements present in the compound. In this way, for each element will be found 2 relations for each flow generated.

The compositions at the ends of the column shows the separation of the two components included in the mixture entered the system allowing to achieve the objective of the process for purification and separation of the components. At the same time the linearity of the system can be observed starting from the analysis of the temperatures conserved in each one of the plates.

The compositions obtained in the process would allow the production of the propylene at polymer grade and propane ready to be distributed to a home, vehicular network or to be reused in the system.

The type of distillation presented shows advantages, due to the high efficiency that allows obtaining for a maximum performance, directly impacting the operating costs allowing their reduction, on the other hand, this type of columns was easy to use taking into account only it was necessary to maintain the conditions of operation, which were easy to follow.

REFERENCES

[1] Plaza, M.G., A.F.P. Ferreira, J.C. Santos, A.M. Ribeiro, U. Müller, N. Trukhan, J.M. Loureiro and A.E. Rodrigues, 2012. "Propane/propylene separation by adsorption using shaped copper trimesate MOF," *Microporous Mesoporous Mater.*, 157: 101-111.

[2] Helton, K., 2012. *Industrial Processes*, First.,

[3] AFSARMANESH, H., 2010. "A reference architecture for scientific virtual laboratories," *Elsevier*.

[4] Granato, M.A., T.J.H. Vlugt and E. Rodrigues, 2010. "Potential Desorbents for Propane / Propylene Separation by Gas Phase Simulated Moving Bed : A Molecular Simulation Study," *Adsorpt. J. Int. Adsorpt. Soc.*, pp: 5826-5833.

[5] Shahandeh, H., J. Ivakpour and N. Kasiri, 2014. "Internal and external HIDiCs (heat-integrated distillation columns) optimization by genetic algorithm," *Energy*, 64: 875-886.

[6] Suphanit, B., 2011. "Optimal heat distribution in the internally heat-integrated distillation column (HIDiC)," *Energy*, 36(7): 4171-4181.

[7] Nakanishi, T., T. Takamatsu, M. Nakaiwa, K. Aso, H. Noda and N. Kuratani, 2009. "A case study of HIDiC design and energy saving," *Comput. Chem. Eng.*, 23: S855-S858.

[8] Kiss, A.A. and Ž. Olujić, 2014. "A review on process intensification in internally heat-integrated distillation columns," *Chem. Eng. Process. Process Intensif.*, 86: 125-144.

[9] Kansha, Y., N. Tsuru, C. Fushimi, K. Shimogawara and A. Tsutsumi, 2010. “An innovative modularity of heat circulation for fractional distillation,” *Chem. Eng. Sci.*, 65(1): 330-334.
[10] Benali, M. and B. Aydin, 2010. “Ethane/ethylene and propane/propylene separation in hybrid membrane distillation systems: Optimization and economic analysis,” *Sep. Purif. Technol.*, 73(3): 377-390.
[11] Ho, T.-J., C.-T. Huang, J.-M. Lin and L.-S. Lee, 2009. “Dynamic simulation for internally heat-integrated distillation columns (HIDiC) for propylene–propane system,” *Comput. Chem. Eng.*, 33(6): 1187-1201.
[12] Suphanit, B., 2010. “Design of internally heat-integrated distillation column (HIDiC): Uniform heat transfer area versus uniform heat distribution,” *Energy*.
[13] Yildirim, Ö., A.A. Kiss, and E.Y. Kenig, 2011. “Dividing wall columns in chemical process industry: A review on current activities,” *Sep. Purif. Technol.*, 80(3): 403-417.
[14] Caballero, J.A., 2015. “Logic hybrid simulation-optimization algorithm for distillation design,” *Comput. Chem. Eng.*, 72: 284-299.
[15] Li, X. and W. Yu, 2011. “Modeling and neuro control for multicomponent nonideal distillation column,” *IEEE Int. Conf. Control Autom. ICCA*, pp: 979-984.
[16] Shahandeh, H., J. Ivakpour and N. Kasiri, 2014. “Internal and external HIDiCs (heat-integrated distillation columns) optimization by genetic algorithm,” *Energy*, 64: 875-886.
[17] Wang, L., M. Kano and S. Hasebe, 2009. “Effect of Multiple Steady-States on Operation Strategy and Control Structure for a Heat Integrated Distillation Column (HIDiC),” in *Computer Aided Chemical Engineering*, 26: 447-451.
[18] Cong, L., L. Chang and X. Liu, 2015. “Nonlinear-wave based analysis and modeling of heat integrated distillation column,” *Sep. Purif. Technol.*, 150: 119-131.
[19] Sadeghifar, H., 2015. “Simple and rapid determination of effective Murphree component efficiencies for operating absorbers, strippers and distillation columns filled with any type of plates,” *Sep. Purif. Technol.*, 139: 104-108.
[20] Kapoor, U., A. Rani, V. Singh and J.R.P. Gupta, 2011. “Simulation and Control of Reactive Distillation Column,” *Power Electron. (IICPE), 2010 India Int. Conf.*, pp: 1-7.
[21] de Hemptinne, J.-C., J.-M. Ledanois, P. Mougin and A. Barreau, 2002. *Select Thermodynamic Models for Process Simulation - A Practical Guide using a Three Steps Methodology*, FIRST EDIT. PARIS, FRANCIA: Technip.
[22] Elgue, S., L. Prat, M. Cabassud, J.M. Le Lann and J. Cézerac, 2004. “Dynamic models for start-up operations of batch distillation columns with experimental validation,” *Comput. Chem. Eng.*, 28(12): 2735-2747.
[23] Vanaki, A. and R. Eslamloueyan, 2012. “Steady-state simulation of a reactive internally heat integrated distillation column (R-HIDiC) for synthesis of tertiary-amyl methyl ether (TAME),” *Chem. Eng. Process. Process Intensif.*, 52: 21-27.
[24] Jones, J.C., 2012. *Hydrocarbons - Physical Properties and their Relevance to Utilisation*, First edit. JONES & VENTUS PUBLISHING APS.
[25] Karami, G., M. Amidpour, B.H. Sheibani and G.R. Salehi, 2015. “Distillation column controllability analysis through heat pump integration,” *Chem. Eng. Process. Process Intensif.*, 97: 23-37.
[26] Nakaiwa, M., K. Huang, A. Endo, T. Ohmori, T. Akiya and T. Takamatsu, 2009. “Internally Heat-Integrated Distillation Columns: A Review,” *Chem. Eng. Res. Des.*, 81(1): 162-177.