# MODELING AND SIMULATION OF THE DISTILLATION COLUMN PLATES

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#### ABSTRACT

In this paper, we developed the modeling and simulation of different phenomena produced in the plates of a distillation column. We used bond graph tool and SYMBOLS (System Modeling Bond graph Language Simulation) software. Among the various kinds of plates, we chose the distillation column that is available in the department of technology process engineering at the University of Setif (UPO3A). The system to be modeled has a nonlinear behavior due mainly to the coupling of the different phenomena of different natures. We are indeed in presence of hydraulic, chemical and thermal energy. So the elaboration of the graphical model or the analytical one is very difficult. The working of the plates is to assure a thermodynamic balance within the column. After modeling, a SYMBOLS software validate and simulate the phenomena that occur in the plates. In the simulation results, the representation of the chemical potential, temperature, molar flow and pressure of the liquid and steam phases in the column plates justified the operating of the distillation column. Results demonstrated the feasibility of simulating multicomponent distillation under unsteady state conditions with fairly good success. Further improvements were suggested for a better accuracy.

# KEYWORDS

Bond Graph Tool, SYMBOLS Software, Distillation Column, Plates, Modeling, Simulation

# **1. INTRODUCTION**

The systems in process engineering are controlled by the mutual interaction of several phenomena of various natures associating technological components. The modeling implies itself in a step of system study to get qualitative and quantitative information on its behavior and its performances, this in all abstraction of the real system. [1], [2]

Distillation is the process most commonly used in industry to separate chemical mixtures; its applications range from cosmetic and pharmaceutical to petrochemical industries. The equipment required to perform the distillation process is known as distillation column. [3], [4]

Since initial investment and maintenance costs for distillation columns are very high it is necessary to have an appropriate mathematical model that allows improving the comprehension of the column dynamics, especially its thermal behaviour, in order to enhance the model and safety of the process. [5]

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 [6]

Distillation column is defined as a device used to separate components of a mixture using the thermodynamic properties of the components [7].

This solved the problem of nonlinearity to a great extent. There was no direct control for purity. They suggested more study for more advanced model predictive control to reduce the complexity of the system. The bond-graph tool has a multidisciplinary vocation and appears to be the most

adapted for the knowledge of such systems. It permits by its graphic nature with the help of a unique language, to put in evidence the nature of the power exchanges in the system, such as the phenomena of storage, transformation and dissipation of energy. [8], [9]

The main objective of this paper is to model the plates and to simulate phenomena in a distillation column by Bond-graph. Using the software «SYMBOLS» makes the modeling of these elements easier.

# **2. DESCRIPTION OF THE COLUMN** [10], [11]

The distillation is a prime operation in the petrochemical and pharmaceutical industries. It is a chemical process of type column that permits to separate the constituent of a liquid mixture being based on the fact that their boiling points are different.

When a mixture is placed in a surrounding wall under conditions of temperature and pressure as the following:

- Increase of the temperature with a constant pressure,
- Reduction of the pressure with a constant temperature,
- Simultaneous variation of the pressure and the temperature.

Two different phases appear, liquid and steam phase. Thermodynamic balance is established between them.

The set of the installation of the column (Figure 1) is composed by ring in which has occurred liquid and steam contact horizontally with the disposed plates in the column or by garnishing. The superior bottom and the lower bottom are welded to the collar.

The condenser is a device of temperature dissipation; it has for role to condense completely or partially the steams of the column top in order to have the ebb that permits to initiate the liquid current on the plate.

The boiler permits to spray the liquid bottom of the column partially to initiate a current steam inside this one. The ball of ebb allows increasing the debit of ebb, therefore the internal debits of liquid.

The column of distillation consists in a contact of current steam and liquid in the goal to do a transfer of mass between the two phases. However, a contact is generally done by a set of plates. In a normal operating, there is a certain quantity of liquid on every plate, and some arrangements are made to make bring up steam while passing through the liquid, generally by the use of the perforate plates.

A thermodynamic balance has the tendency to settle on every tray, around the surface of contact between the quantities of liquid and steam that there is kept.

We distinguish two zones in a continuous column:

- The zone of rectification (or concentration) is the set of plates situated above the plate of food.
- The zone of weariness is the set of plates situated below the plate of food.

In return for a sufficient number of the successive flashes, we succeed in getting a distillate essentially containing the light compounds and a residual essentially containing the heavy compounds.



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Figure 1. Distillation Column

In a column, the different kinds of plates play a very important role; they are designated to do the transfer of matter between the liquid and steam phases.

Any plates were nourished at a time by two fluxes that are the retiring steam of the lower plate and the liquid coming of the upper plate (Figure 2).



Figure 2. Transfer of matter between the liquid phase and vapor

## **3. MODELING OF THE COLUMN** [12], [13], [14]

A plate is modeled with the help of the incoming fluxes,  $L_{i+1}$ ,  $V_{i-1}$  liquid and vapor coming from the upper and lower plate respectively and retiring  $L_i$  and  $V_i$  of the same i plate.

#### 3.1. Mass balance

The equation of mass conservation permits to write:

$$\frac{dM}{dt} = \Delta L + \Delta V \tag{1}$$

Where  $\Delta L$  is input liquid - output liquid and  $\Delta V$  is input steam - output steam. From the equation (1) and the fractions of the liquid as well as steam we get:

$$M_{j} \frac{dx_{ij}}{dt} = L_{j-1} X_{j,i} - L_{j} X_{j,i} + V_{j+1} Y_{i,j+1} - V_{j} Y_{i,j}$$
(2)

This equation allows us to separate the balances of liquid and steam as follows:

$$\frac{du_{i,j}^{l}}{dt} = L_{j-1}X_{i,j-1} - L_{j}X_{i,j} - LV_{i,j}$$
(3)

$$\frac{du_{i,j}}{dt} = V_{j+1}Y_{i,j+1} - V_{j}Y_{i,j} - LV_{i,j}$$
(4)

Where  $LVj = V_{j+1} - V_j$ 

The bond-graph model of these two parts is given by (Figure 3).



Figure 3. Bond-graph model of the liquid and steam

# 3.2. Energy balance

The equation of energy conservation permits to write:

$$\frac{d(Holdup - Energy)}{dt} = \Delta E_{in} - \Delta E_{out}$$
(5)

Where  $\Delta E_{in}$  and  $\Delta E_{out}$  are the ratio of the input and output energy respectively.

$$\frac{du_{j}}{dt} = h_{i,j-1}^{l} l_{j-1} + h_{i,j+1}^{v} v_{j+1} - h_{i,j}^{l} l_{j} - h_{i,j}^{v} v_{j}$$
(6)

This equation can be written for every state (steam and liquid) as follows:

$$\frac{du_{j}^{l}}{dt} = h_{i,j-1}^{l} l_{j} - h_{i,j}^{l} l_{j}$$

$$\frac{du_{j}^{v}}{dt} = h_{i,j+1}^{v} v_{i+1} - h_{i,j}^{v} v_{j}$$
(8)

Where :  $M_{lj}(t)$  : Residual liquid in the plate lj [mol].  $L_{lj}(t)$  : 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].  $V_{lj-1}(t)$  : Steam flow from the lower plate [mol/s].  $h_{lj}(t)$  : 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].  $H_{lj+1}(t)$  : Enthalpy of the steam from the bottom plate [J/mol].

The corresponding bond graph model is given by (Figure 4).



Figure 4. Bond graph of the energy balance

#### 3.3. Thermodynamic balance

For every constituent i, the thermodynamic balance was given by the following equation:

$$\mu_i^l(t_i, p_i, x_{i,j}) = \mu_i^y(t_i, p_i, y_{i,j}) \Leftrightarrow y_{i,j} = kx_{i,j}$$
(9)

Where  $\mu_i^1$  and  $\mu_i^v$  are the chemical potential respectively of liquid and vapor

# 3.4. Word bond-graph model of the plate

From the figure showing the supply of the plates, the word bond graph model representing the technological stage of the modeling, consists in constructing the architecture of the system by the assembly of the different subsystems whose base elements are simple processes.



Figure 5. The coupled bond-graph (word bond-graph) model

The representation by a true bond graph can be decomposed in three models representing the three phenomena that occur in the plate (Hydraulic, Chemical and Thermal).

## **3.5. Hydraulic phenomenon**

This phenomenon is a two shapes, liquid and steam, the construction of its model comes back to study the equation of fluid flow.

$$\Delta p + p_{ke} = p_1 - p_2 + p_{pe} - p_f \tag{10}$$

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Where 
$$\Delta p = I \frac{dq}{dt} = \rho \frac{v}{A_0^2} q'; \ p_{ke} = p \Delta x_a = \rho \frac{q L_j^i}{2A \mu D_j^i}; \ Pe = \rho g (h_1 - h_2) = \rho g (z_i - h_{j+1}^i)$$



Figure 6. a- Bond-graph of liquid

b- Bond-graph of steam

The global hydraulic phenomenon is represented by (Figure 7) under this two aspects liquid and steam.in which a junction (0) must be added.

The development of the equation (10) gives:

$$\Delta p + p_{dc} + p_{pe} = p_j - p_{j+1} + \rho g (zj - h_{j+1}^l)$$
(11)



Figure 7. Bond-graph model of hydraulic phenomenon

#### 3.6. Thermal phenomenon

We construct the bond-graph model of thermal phenomena (Figure 8) from word bond-graph model after decoupling.

$$Sf_{1} \qquad \begin{array}{c} T_{J}^{L} \\ T_{J}^{L} \\ Sf_{1} \\ \vdots \\ Sf_{2} \\ \vdots \\ Sf_{2} \\ Sf_{2} \\ Sf_{2} \\ \vdots \\ Sf$$

Figure 8. Bond-graph model of the thermal phenomenon

## **3.7** Chemical phenomenon



Figure 9. Bond-graph model of the chemical phenomenon

## 4. SIMULATION OF THE COLUMN PLATES PHENOMENA

We made an experience in the laboratory of engineering chemistry (industrial chemistry department UFAS), where we saw the operation of distillation of a binary mixture (water + methanol) with the distillation column (UPO3A).

The simulation of our system resides in the representation of the parameters (chemical potential, temperature, molar flow and pressure) of the liquid phase and steam in the plate of a column to distill. [15]

The results of simulation on SYMBOLS software are illustrated below by the represented figures.

#### 4.1. Chemical potential

The figure 10 gives the evolution of the chemical potentials of the liquid phase and phase steam. We note that the chemical potential increases in exponential manner; this increase is attributable to the increase of liquid-steam contact in the plates.



Figure 10. Chemical potential of liquid and vapor evolution

## 4.2. Molar flow

The evolution of the molar fluxes of the liquid phase and the steam phase is given by the figure 11. The molar flow of the liquid (resp. of steam) decreases logarithmic way of 4.5 [mole/min] to 0.54 [mole/min] (resp. of 2.95 [mole/min] to 0.30 [mole/min]). The variation of the molar flows is a reason of reduction of the number of moles of the liquid in the mixture (resp. of steam).



Figure 11. Molar fluxes of liquid and steam phases

## 4.3. Temperature and entropy flow

The evolution of the temperatures and the fluxes of entropy in a tray of the column are given by the figure 12:



Figure 12. Variation of the temperature and the entropy flow

We note that the temperature of the liquid phase and phase steam in a tray of distillation is equal. The temperature evolves exponentially according to time; it is due to the phenomenon of energystorage. In our example, to t =5mn the temperature becomes steady what leads the mixture toward a thermodynamic balance state. The flow of entropy varies to the inverse sense that the temperature.

# 4.4. Pressure

The evolution of the pressure of a tray is given by the figure 13 :



The curve representing the pressure follows an exponential law according to the time. It verifies the empiric equation well; this variation is due to the heap of the matter of a tray. In our example, to t = 5mn the pressure becomes steady, what leads the mixture in a thermodynamic balance state.

# 4. CONCLUSION

In this paper, we achieved a model of essential part of discontinuous distillation column namely the plates. We saw that are essential elements of the column since they assure liquid-steam contact.

On these active elements of the column, they produced hydraulic, chemical and thermal phenomena during the separation between liquid and steam phases. This model has been validated by the use of the software SYMBOLS. The results were satisfactory, since we simulated some processes with the corresponding parameters to another modeling, and we got similar results and in conformity with the specifications.

The analysis of the results gotten permitted to put in evidence the evolution of the variables of state of the system during the time. This analysis permitted to understand the dynamic aspects of the better system.

The bond-graph tool and the software proved to be powerful and convenient means for this project that consisted of the modeling, the simulation and the analysis of the results.

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