A MODELLING METHODOLOGY FOR DISTILLATION COLUMNS USING DYMOLA AND SIMULINK

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Abstract

In this paper we present a modelling methodology for distillation columns, which allows modelling the ideal column for a well-known mixture. The methodology combines three steps; a first step where are calculated all necessary data to build the model. A second step, where four types of sub-models and the control strategy are properly connected using Dymola or Simulink. And the third step where the controllers are tuned using simulation data.

The methodology has provided good results with different mixtures (for example: water and acetic acid, water and acetone, water and methanol) in several operation conditions. Besides it has been useful to get a good benchmark of distillation columns models. These models are being used for multivariable control evaluations and will be integrated into a virtual laboratory for training students about the distillation process and its control.

Key Words

Modelling, Simulation, Control of Complex System, Process Control, PID control, Industrial Processes

1. Introduction

Distillation is a complex process that involves large and interesting modelling and control problems [1], [2], [3]. This paper collects the experience of the authors in both fields when they tried to model binary distillation columns (see Fig. 1) with inventory control, using general modelling languages as Dymola and Simulink instead of industrial dynamic simulation packages such as Aspen-Plus or Hysis.

The modelling should be modular and rigorous [4], therefore it was selected an EMC staged structure [5] that includes a non-null dynamic balance of material, composition and energy in each equilibrium stage. In order to limit its complexity, assumptions like "negligible vapour hold-up" and "vapour flow up the column equal on all trays", very usual in the design of industrial distillation columns, should be incorporated in the model. Further the modelling should also consider the design of the appropriate column to distillate the mixture in the operation conditions selected by the user, so an integrated modelling methodology looks adequate.

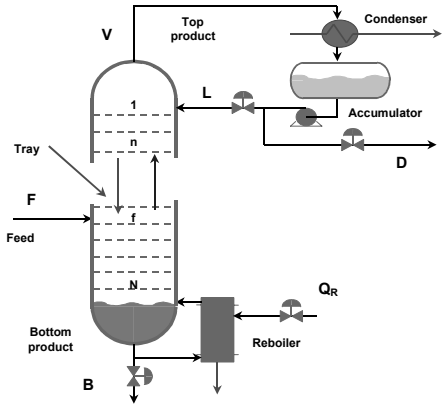

Figure. 1. Distillation Column

In section 2 of this paper are described the concrete features of the staged model. In section 3 the modelling methodology, which takes advantage of the modular modelling, is presented. This methodology has been tested efficiently in some mixtures, an example is described in the section 4.

2. Features of the Staged Model

It is generally agreed that the staged models [4] describe real trayed columns very well. In this paper the columns are modelled combining five modules in order to get reusability and generality. The first and more important module is the conventional tray. This module will be repeated so many times like trays minus one there are in the column. The other modules are the feed tray, the top group, the bottom group and the controller (one for the top group and one for the bottom group).

All modules except the controller are modelled as equilibrium stages using three groups of equations: (1) the differential equations describing the dynamic behaviour of the main variables (mass, composition and temperature), (2) the algebraic equations describing the hydraulic relations between the mass, the liquid flow and the vapour flow and (3) the liquid-vapour equilibrium equations. The main equations are mentioned in the following sections, with special attention to the conventional tray. Its hypotheses and simplifications will be a good reference for the other modules. The nomenclature of the variables is attached at the end of this paper.

2.1. Conventional Tray

<u>*Dynamic behaviour:*</u> (See Fig. 2)

Overall material balance.

$$\frac{dM_n}{dt} = L_{n-1} + V_{n+1} - V_n - L_n \tag{1}$$

Balance of the light component's composition.

$$M_n \frac{dx_n}{dt} = (x_{n-1} - x_n)L_{n-1} + (y_{n+1} - x_n)V_{n+1} + (x_n - y_n)V_n \tag{2}$$

Energy balance.

$$M_n \frac{d(T_n)}{dt} = (T_{n-1} - T_n)L_{n-1} + (T_{n+1} - T_n)V_{n+1} \tag{3}$$

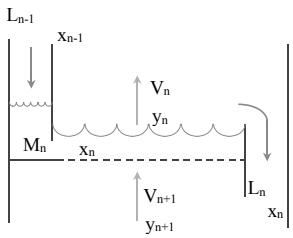

Figure. 2. Column Tray

The energy balance, which appears as function of the temperature, is consequence of using the liquid and vapour enthalpy equations of [5] and the following hypotheses: a) the heat capacity and the heat of vaporization of the mixture for two near stages are very similar, b) the vapour flow up the column is equal on all trays (used with good results in the 95% of industrial columns models, [2]).

<u>*Hydraulic relations:*</u>

$$L_n = \frac{M_n}{\tau} - \lambda V_n \tag{4}$$

$$V_n = V_{n+1} \tag{5}$$

The relation (4), [6], assumes that the liquid flow, which arrives to a stage, depends on the vapour flow, which leaves the stage, and of the retained mass in this stage. The relation (5) assumes that vapour flow is equal on all trays, mentioned before, so the vapour flow along the column is the vapour flow generated in the bottom.

<u>*Liquid-Vapour Equilibrium*</u>:

Antoine's Law for each component, i or j.

$$\log_{10}(P_n^s) = A_{i,j} - \frac{B_{i,j}}{C_{i,j} + T_n} \tag{6}$$

Dalton's Law.

$$P_n = \gamma_{n_i} x_{n_i} P_{n_i}^s + \gamma_{n_j} x_{n_j} P_{n_j}^s \tag{7}$$

Raoult's Law for the light component.

$$y_{n_i} P_n = \gamma_{n_i} x_{n_i} P_{n_i}^s \tag{8}$$

Van Laar's equations.

$$\ln(\gamma_{n_i}) = A_{12}\left(\frac{A_{21}(1-x_{n_i})}{A_{12}x_{n_i} + A_{21}(1-x_{n_i})}\right)^2 \qquad \ln(\gamma_{n_j}) = A_{21}\left(\frac{A_{12}x_{n_i}}{A_{12}x_{n_i} + A_{21}(1-x_{n_i})}\right)^2 \tag{9}$$

The inclusion of the activity coefficients γ [5], [2] in (7) and (8), and the Van Laar's equations [7] that calculate them, have been necessary to consider non-ideal mixtures.

2.2. Feed Tray

Due to the feed flow, the liquid flow in the stripping section is bigger than in the other section of the column. Therefore, the feed tray is modelled like a conventional tray, but including a term referring to the feed in the three differential equations. The following hypothesis has been also considered: the temperature of the feed is the same as the boiling temperature of the mixture and similar to the temperature of the feed tray.

2.3. Top Group

The energy balance in the top group (See Fig. 3), given by (10), is similar to the equation (3), with an additional term taking into account the heat losses (Q_c) in the condenser. Therefore, it is necessary another expression (11) to calculate these losses. The hypothesis "the heat capacity

and the heat of vaporization of the mixture for two near stages are considered very similar" is used again.

$$c_D M_D \frac{d T_D}{dt} = c_D V_1 (T_1 - T_D) + H_1^{VAP} V_1 - Q_c \quad (10)$$

$$Q_c = (c_D T_1 + H_1^{VAP}) V_1 - c_D T_D (L + D) \quad (11)$$

In order to model the exit flows (the reflux flow and the distilled flow) of the top group, it is assumed that the accumulator is a deposit with two valves and thus, whatever comes out of its exit valves will be proportional to the square root of the mass that retains.

$$L = A_L K_L \sqrt{M_D} \qquad D = A_D K_D \sqrt{M_D} \quad (12)$$

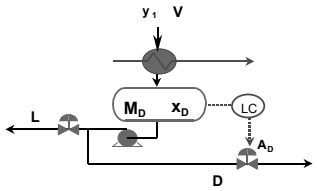

Figure 3. Top Group

2.4. Bottom Group

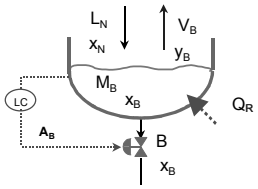

Figure 4. Bottom Group

The modelling of this group (See Fig. 4) assumes that the bottom of the column is also as a deposit. So, the bottom flow depends on the retained mass in the bottom by the expression:

$$B = A_B K_B \sqrt{M_B} \quad (13)$$

The energy balance in this stage, given by (14), is similar to the equation (3), with an additional term referring to the heat flow (Q_R). Therefore, it is necessary another expression to calculate the initial vapour flow (V_B). It is calculated, see equation (15), from the energy equilibrium between the heat flow and the energy flows that go through the stage.

$$c_B M_B \frac{d(T_B)}{dt} = (T_N - T_B) c_B L_N - H_B^{vap} V_B + Q_R \quad (14)$$

$$Q_R = H_B^{vap} V_B + T_B c_B B - T_N c_N L_N \quad (15)$$

3. The Modelling Methodology

The number of theoretical stages, N, and the parameters for the flow dynamics are often obtained by matching plant data [4]. However, this section approaches a different problem; given a two-product mixture, how must be modelled a column able to distillate it?, which data are need? A three steps modelling methodology, which takes advantage of the staged model presented in section 2, is proposed.

- *First step*: The column design, where all necessary data to build the model are calculated. The user takes active part in the column design, collecting the data and selecting the operation conditions. A list of these data is shown on the left column of Table 1, whereas the right column of Table 1 shows the calculated variables.

- *Second step*: Building the model, where the elemental blocks, described in section 2, and the control strategy (optional) are properly connected.

- *Third step (optional)*: Tuning the controllers, where the two PID controllers are properly tuned using simulation data.

After these steps, the user of the modelling methodology can simulate the wanted distillation process. The simulation will start from a steady-state, characterized by the following variables: masses in accumulator, bottom and trays, composition and temperature in each stage, valve openings, feed flow, composition and temperature of the feed, heat flow.

3.1. The Column Design

It is understood that an elemental design consists in "The determination of: the number of trays of the column, the liquid and vapour compositions of the light component's in each tray, the temperature in each tray, the position of the feed tray, the initial liquid and vapour flows, and the initial bottom and distilled flows". But the proposed column design (see Table 1) includes more calculations than the elemental design.

As traditional design method has been selected the McCabe Thiele's method [1]. Its automation has need the polynomial fit of the equilibrium curve (the first calculation of the Table 1) and the request to the user of the data mentioned in the second row of the Table 1.

Between the additional calculations deserve special mentions the determinations of: the parameters (λ, τ) of the hydraulic equation, the initial retained masses in the accumulator, trays and bottom (M_D, M_n and M_B), and the constants K_B, K_D and K_L of the valves.

A data form has been defined in order to help the user in the column design. And a Matlab program has been developed in order to semi-automate the design. Some data of the form has a great influence in the column design; changing them the user can design several columns with different dimensions or different behaviour for a same mixture. Four variables (the composition of feed, top product, bottom product and the ratio L/D) have direct influence in the number of trays and the position of the feed tray. Other variables (the feed flow, the volume of the trays, accumulator and bottom) have direct influence in the dynamic of the column.

KNOWN VARIABLES	**CALCULATED VARIABLES**
Selected mixture Equilibrium curve of the mixture (x-y-T)	Polynomial of the equilibrium curve
Feed flow (F) Composition of the light component in liquid phase in the feed (x_f) Composition of the light component in liquid phase in the top group (x_D) Composition of the light component in liquid phase in the bottom group (x_B) Initial relation of external reflux (L/D)	Reflux flow (L) Vapour flow (V) Distilled flow (D) Bottom flow (B) Number of theoretical stages (N) Feed tray position (x-y-T) for each tray
Boiling temperature of the two components (^oC) Density of the two components (g/cm^3) Molecular weight of the two components (g/mol) Composition of the light component in liquid phase in the mixture (%)	Temperature of the feed flow (T_f) Density of the mixture (g/cm^3) Molecular weight of the initial mixture (g/mol) Molecular weight of the mixture in the top and bottom groups Number of mole in a litre of mixture
Volumes (l) of the accumulator, bottom and trays	Initial retained masses in accumulator, bottom and trays (mole) (M_D, M_n and M_B) Parameters of the hydraulic equations (λ and τ (s)) Valve constants (K_D, K_L and K_B) with valve openings (A_D, A_L and A_B) at 50%
Heat capacity of the two components (cal/g^{o}C) Heat of vaporization of the two components (cal/g)	Heat capacity of the top and bottom groups. (c_D y c_B) Heat of vaporization of the top and bottom groups (H^{vap}_D y H^{vap}_B) Heat flow (cal/s) (Q_R)
Antoine's coefficients [$A_{A,B}$, $B_{A,B}$, $C_{A,B}$] Van Laar's constants [A_{12} A_{21}]	
Name of the file, where all these data are saved	File *.mat

Table 1: Variables of the Column Design

3.2. Building the Model

The staged model can be built with or without the inventory control, connecting the following elemental blocks: so many conventional tray sub-models as number of trays minus one there are in the column, a feed tray sub-model, a top group sub-model, a bottom group sub-model, two digital PID controllers and auxiliary blocks in order to can manipulate the two or four free valves. The model can be built in Dymola or Simulink because all the sub-models have been developed in the both languages (In [10] all of this sub-models are developed in detail).

The modelling in Dymola is made with two text files, the first (*.dym) including a declaration for each block and the connections between them, the second (*.dyc) including the call to the file (*.dym), the call to equations ordering and the initialisation of variables. The modelling in Simulink is made graphically into a file (*.mdl) copying the blocks, connecting them and filling his masks. It is advisable to use Dymola when the number of the trays in the column is very high. Otherwise, when the model has only a few trays or when the user wants to test different control strategies on a given column, it is more appropriate to use Simulink.

Some examples of how to build the model of a column in Dymola and Simulink are developed for different mixtures in [10].

3.3. Tuning the Controllers

It is very usual that the distillation columns are modelled with an inventory control strategy, which tries to maintain the levels or the masses in the accumulator and in the bottom. There are twelve possibilities of do it [2] in the

column of Figure 1, but the most common way is shown in Figure 3 and 4; the mass in the accumulator is controlled with the distilled flow and the mass in the bottom with the bottom flow.

When the user builds the model, he can connect any inventory control strategy or none. Then he must tune the controllers, he should make simulations with the two controllers in manual mode and to study the behaviour of the retained masses in the accumulator and the bottom, when the valve openings vary. These behaviours are analysed with another Matlab program, which calculates a matrix (2x2) of transfer functions. With that matrix and the multivariable control tool developed by [8], the user can analyse the interactivity and get the appropriate control parameters.

4. Example

A non-ideal binary mixture of water and acetic acid has been chosen to show the proposed methodology. The water is the light component of the mixture with a boiling temperature of 100ºC. The acetic acid is the heavy component with a boiling temperature of 118.3ºC. The equilibrium curve x-y-T (liquid and vapour composition of the light component, and temperature at 760 mm Hg), and the other features of the mixture has been obtained from [7] and [9].

The column design determines 18 trays to operate in the following conditions: [F= 20 mole/s; x_F= 0.5 %; x_D= 0.9 %; x_B= 0.002 %; L/D= 3]. Also, the program determines [λ= -0.75; τ= 9.87s; M_D = 1302 mole; M_B = 1348 mole; Q_R= 350730 cal/s] as consequence of the following volumes and valve openings [Vol_D=100 litres; Vol_B=100 litres; Vol_n=50 litres; A_D= 50%; A_L= 50%; A_B= 50%]. At last, the control parameters obtained for the most common inventory control strategy are the following: (K_P = - 0.08, T_I =128, T_D = 0) for the top and (K_P = - 0.28, T_I = 246, T_D = 0) for the bottom.

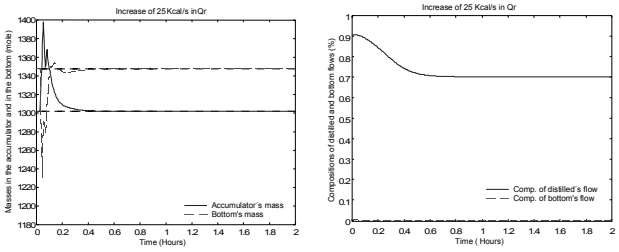

Figure 5. Evolution of Masses and Compositions in the Top and in the Bottom, with a Positive Change in the Heat Flow

Next the column's model with the inventory control strategy has been tested. Figure 5 shows the behaviour of the masses in the accumulator and in the bottom and the compositions in the distilled and bottom flows, when the heat flow in the bottom changes from 350730 to 375730 cal/s. In Figure 6, one can observe the responses when the reflux flow changes, opening its valve from 50% to 55%. In both experiments, the masses of the accumulator and of the bottom recover the initial values, due to the actions of the PID controllers, whereas the compositions move to new values.

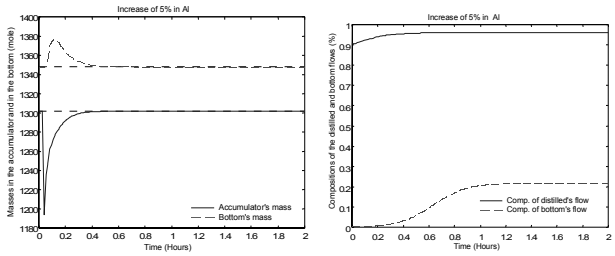

Figure 6. Evolution of Masses and Compositions in the Top and in the Bottom, with a Positive Change in the Reflux Opening

5. Conclusions

The paper proposes a methodology to model and simulate a distillation column for a given mixture, ideal or non-ideal, given the equilibrium curve of the mixture and a few specifications. The modelling goes further than a dynamic modelling, since it includes the column design and the tuning of the controllers. The methodology takes advantage of modular structure, using five sub-models developed in Dymola and Simulink.

The methodology has been tested efficiently in some mixtures (water and acetic acid, water and acetone, water and methanol) [10]. Though only an example has been described due to space limitations. Besides it has been useful to get a good benchmark of distillation columns models. These models are being used for multivariable control evaluations and will be integrated into a virtual laboratory for training students about the distillation process and its control.

6. Acknowledgements

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7. Nomenclature

B, bottom flow

c, heat capacity of mixture

D, top product/distilled flow

F, feed flow

H^{vap}, heat of vaporization of mixture

L, liquid flow or reflux flow

M, retained mass

N, number of theoretical stages

Q_C, heat losses in the condenser

Q_R, heat flow

T, temperature

x, composition of light component in liquid phase

y, composition of light component in vapour phase

V, vapour flow

Vol, volume

γ activity coefficient

τ, hydraulic constant time

λ, K2- effect

A_{12}, A_{21}, Van Laar's constants

$A_{i,j}$, $B_{i,j}$, $C_{i,j}$, Antoine's coefficients

A_L, A_D, A_B, valve openings

K_L, K_D, K_B, valve constants

K_P , T_I, T_D, control parameters

Superscripts:

S, saturation;

Subscripts:

B, bottom

D, distilled

F, feed

i, j, component i or j

N, last stage

n, study stage

n-1, previous stage

n+1, next stage

1, first stage

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P, pressure

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