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PRACTICAL ASPECTS IN MODELLING AND CONTROL OF RECTIFYING COLUMNS

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Abstract: This paper presents a study of practical aspects regarding the design of control systems for rectifying columns: choosing the position of temperature sensors on the column, choosing the pairs sensors-control variables, choosing the adequate control structures and instability problems that can occur in these structures.

Key words: rectifying columns, control system, temperature sensors.

1. INTRODUCTION

The rectifying processes are the most used to separate the liquid mixes. These processes consist of multiple vaporisation-condensation operations and take place in complex installations as tray or packing columns. The tray-type distillation columns usually have a great number of trays (in the magnitude of tens) and the mathematical modelling and simulation represent a huge challenge for the controller and programmer. The mathematical model consists of n x 3 first order non-linear differential equations (three for each tray and n is the number of trays), plus the models of other equipment attached to the column. This model is completed with several algebraic equations describing the relations between the state variables for the process (usually flows, concentrations and temperatures) and the other dependent variables that characterize the binary system (liquid-vapours) existing on each tray [7, 9]. The vaporisation-condensation processes in the column are taking place at equilibrium, thus any pressure change lead to changes in the boiling temperature. These changes are modifying the internal energy of the system that transforms in evaporation heat. Thus the mathematical modelling shall consider both mass transfer and energy transfer that are taking place in the system. The vapour flow (V), from column base to the top, and the liquid flow (L) from top to the bottom generate the mass and energy transfer, both ways, inside the column.

Besides all these technological problems, new problems are generated by the selection and installation of sensors used to collect information regarding the system operation such as:

- impossibility of on-line measurement of concentration on key trays due to lack of real time concentration sensors and the substitution of concentration measurements with temperature measurements;
- the placement of sensors on the column shall permit the detection of perturbations in the liquid-vapour equilibrium;
- the number of sensors for estimation of the temperature and pressure profiles in the column shall be small due to construction issues.

All these problems lead to the necessity of a systematic study of the technological process that takes place in the column, before all other activities regarding the modelling, simulation and design of the control system.

2. BASIC CONTROL

The figure 1 presents the simplified technological diagram of a rectifying column, showing the actuators placed on the flows that can be used as control variables, such as: F_R – Flow rate of reflux; F_B – Flow rate in the bottom; Q_B – Flow rate in the reboiler; F_D – Flow rate of the distillate; F_C – Flow rate in condenser.

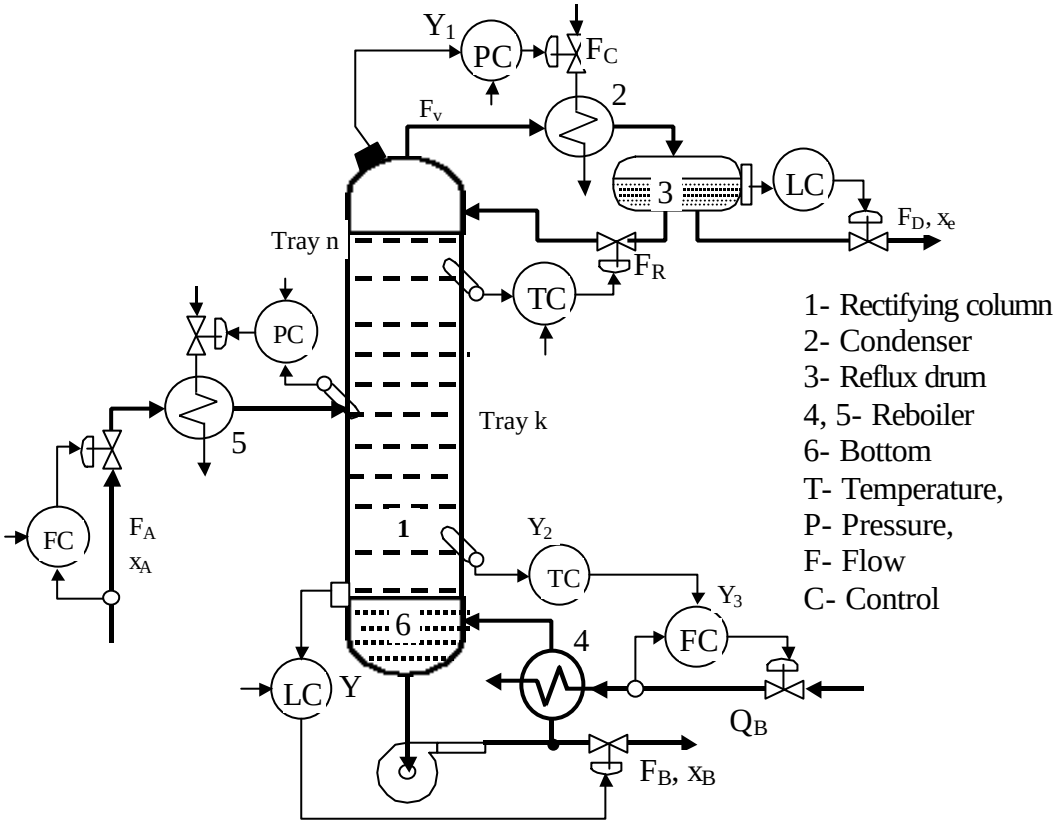

Fig. 1. Basic Column Control

a) Control variables. The number of necessary control variables is given by the number of degrees of freedom for the process [3, 6, 9]. For example, a binary system with two phases (liquid and vapours) has two degrees of freedom (Gibbs relation). Therefore, two out of the five control variables for the process can be used to control the column in order to get the required separation rate, the other three variables being used to satisfy supplementary requirements for system safety.

b) Measured process variables. The basic objective for the control system is to get the highest separation rate for the mix fed into the column through flow F_A, having the concentration of the high volatile component X_A. This requires certain values for the concentrations at the column's top X_e and column's bottom X_B for a given productivity (function of the number of trays). Since on-line concentration sensors are not readily available, temperature sensors are used in order to determine the concentrations using the Raoult and Dalton laws applicable to binary systems. Therefore the pressure profile in the column must be known. It is necessary to carefully choose the pressure sensors in order to guarantee: enough thermocouples located so that the temperature profile can be

determinate, differential pressure measurements to sense flooding, flow measurement of all streams. It is important to include these measurements in the initial equipment design since having to make field modification to an operating column can be very expensive and may take a long time to accomplish [1, 5, 6, 7, 8, 9].

One of the most important issues in column control is to establish an appropriate temperature sensor location, function of the distributed nature of distillation process. The fundamental idea is to control one or more well selected temperatures (for indirect measurement of composition) and to reduce the effect the disturbances. Each stage provides a possible location for a unique measurement to be made. Luyben and Moore [7] offer a good solution for the sensor locations function of the temperature sensitivities.

The sensitivity information can be conveniently summarized in K_{XT} matrix form of the steady-state temperature gain in (1), where: T_j is the temperature on stage j; XCi is the command variable, $(F_R, Q_B,)$ or input perturbation F_A.

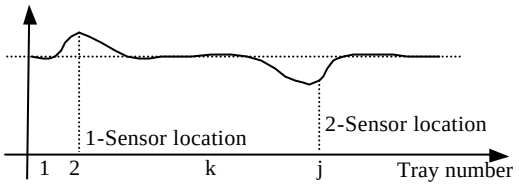

Fig. 2. Sensor location

$$K_{XT} = \begin{bmatrix} \frac{\partial T_1}{\partial X_{C1}} & \frac{\partial T_2}{\partial X_{C2}} \\ \frac{\partial T_2}{\partial X_{C1}} & \frac{\partial T_2}{\partial X_{C2}} \\ \vdots & \vdots \\ \frac{\partial T_n}{\partial X_{C1}} & \frac{\partial T_n}{\partial X_{Cn}} \end{bmatrix} \qquad (1)$$

The numerical values of the matrix K_{XT} are represented in the figure 2 function of the stage number. The trays of the maximum values of K_{XT} indicate the places to locate the control sensors.

*c) **Selecting input-output pairs*** (sensor-valve). The selection of the controlled and manipulated variables defines the structure of control system.

Distillation control systems usual include two levels of focus:

- A first-level concerned with stabilizing the basic operation of the column, named *supply control*, which includes flow controls of the material and energy streams, on the reboiler and accumulator.

- A second-level control addresses the separation-taking place in the column, named *separation control* that includes the control of compositions X_B and X_e, through direct control of temperatures T_a and T_B as an indirect measurement of composition (Temperature sensor is a fast inexpensive sensor).

Usually, the valve F_C is selected for the pressure control. The others, (F_L, F_B, F_D, Q_B) are selected for the supply and separation control, at the top and bottom area of the column. The control engineer must decide which of the valves available for separation control are to be manipulated by the control system and which are to be available for supply control.

In the table 1 are given the possibilities to choose the sensor-valve pairing and the distribution of valves for separation (SP) and supply (SY) control [7].

Table 1. The sensor-valve pairing (corresponding to the fig. 1)

Nr	Control structure	Valve allocation				Control Variables		Control type
		F_D	F_R	Q_B	F_B	Separation	Supply	
1	F_R - Q_B	SY	SP	SP	SY	F_R - Q_B	F_D - F_B	Classic
2	F_D - Q_B	SP	SY	SP	SY	F_D - Q_B	F_R - F_B	Inverse
3	F_R - F_B	SY	SP	SY	SP	F_R - F_B	F_D - Q_B	Special separation
4	F_R/F_D - Q_B	SY	SP	SP	SY	F_R/F_D - Q_B	F_D - F_B	Reflux Ratio Limit.
5	F_R - Q_B /F_B	SY	SP	SP	SY	F_R - Q_B /F_B	F_D - F_B	Bottom evacuation
6	F_R/F_D - Q_B/F_B	SY	SP	SP	SY	F_R/F_D-Q_B/F_B	F_D - F_B	

To select the pair sensor-valve is recommended to use the sensitivity analysis for each pair and to choose the combination with minimum interactions between control loops. The structure of the control system for line 1 in the table is presented in figure 1.

3. COMPUTER SIMULATION.

3.1 Column's dynamic models.

a) Stage model. The distillation stage dynamic model based on the diagram presented in figure 3 consists in following equations [9]:

- Overall mass balance: $$\frac{dM_j}{dt} = L_{j+1} + V_{j-1} - L_j - V_j + F_A \quad (2)$$

- Component mass balance: $$\frac{d\left(x_i M_j\right)}{dt} = x_{i,j+1}L_{j+1} + y_{i,j-1}V_{j-1} - x_{i,j}L_j - y_{i,j}V_j + x_{iA}F_A \quad (3)$$

- Energy balance: $$h_j^L \frac{d\left(M_j\right)}{dt} = h_{j+1}^L L_{j+1} + h_{j-1}^V V_{j-1} - h_j^L L_j - h_j^V V_j + h_A^L F_A \quad (4)$$

$$h_j^L = A_j T_j + B_j T_j^2 \quad , \quad h_j^V = A_j^V T_j + B_j^V T_j^2 + \Delta H_i^V\,(0°C) \quad (5)$$

- Liquid hydraulics (Francis Weir): $L_j = C\rho_j^L w H_0^{1.5}$, $M_j = M_{0j} + \rho_j^L S H_0$ (6)

- Vapour-Liquid Equilibrium: $y_{i,j} = K_{i,j} X_{i,j}$, $K_{i,j} = \frac{\gamma_{i,j} P_{i,j}^S}{P_j}$ (7)

where: H_0 = hold-up of the tray, $P_{i,j}$ = vapour pressure of the component i, M_j = liquid mass on the stage j, $x_{i,j}$ and $y_{i,j}$ = liquid and vapour composition on the stage j.

b) Partitioning of the dynamic model. In order to include in the simulation model the delays that appear in the real operation of the column, it is necessary to partition the equations of the trays according with the simulation structure presented in figure 3.

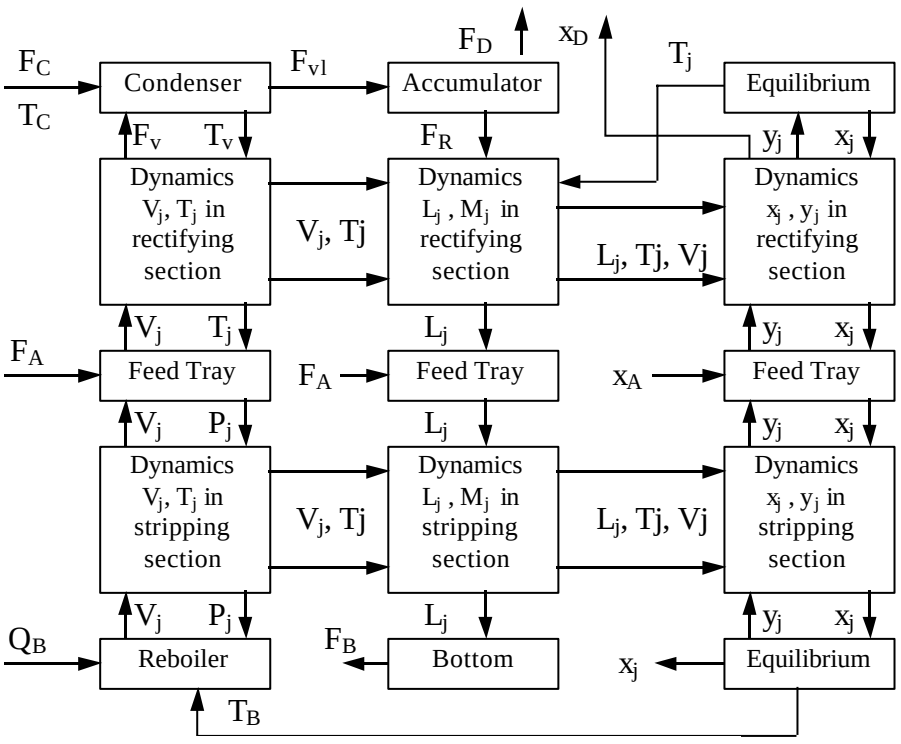

Fig. 3 Partitioning of the dynamic model

The main issue in modelling of the distillation processes is the determination of the

equilibrium temperature T_j for each tray in order to get the enthalpies h_j^L and h_j^V from the energy balance. Therefore, the procedure "Equilibrium" is introduced in the equations of the simulated model to determine the temperature T_j using the mathematical relations for evaporation-condensation processes in multi-phase mixtures:

$$y_i = \frac{g_i P_i^V}{P} \cdot X_i; \quad \text{were vapour pressure is } P_i^V = \exp\left(C_{1,i} + \frac{C_{2,i}}{T + C_{3,i}}\right) \qquad (8)$$

To calculate the equilibrium temperature T_j for a tray:

- Define the convergence function: $f = 1 - \sum x_i$ (9)
- Choose an initial value for temperature T_k corresponding to the given values x_i, y_i.
- Recalculate the temperature using the convergence expression (10):

$$T_{k+1} = T_k + \frac{1}{\sum \frac{\partial x_i}{\partial T}} \cdot f = T_R + \frac{1}{\sum x_i \cdot \frac{C_{2,i}}{T + C_{3,i}}} \left(1 - \sum x_i\right) \qquad (10)$$

3.2 Instability problems in distillation columns control

During the implementation of the automatic control systems for distillation columns, unstable regimes can occur due to sensors and actuators selection and placement. In order to illustrate these aspects, we shall consider a column with only one tray (see figure 4). The mathematical model is determined using equations (2) to (7).

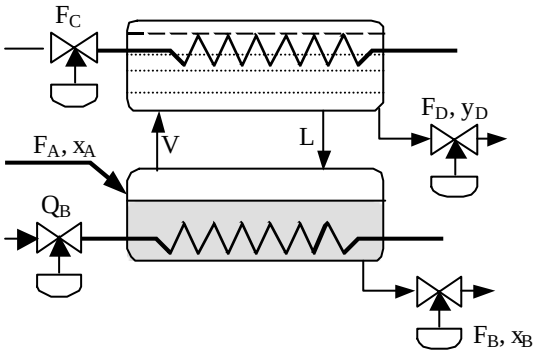

Fig. 4. One tray column

$$M_L \frac{dx_B}{dt} = F_A \cdot X_A - F_B \cdot X_B - F_D \cdot Y_D \qquad (11)$$

$$F_D = V - L, \; F_A + L = V + F_B \qquad (12)$$

The flows V (vapours) and L (reflux) are chosen as control variables. From (11) and (12) we get:

$$M_L \frac{dx_B}{dt} = F_A \cdot (X_A - X_B) + L(Y_D - X_B) - V(Y_D - X_B) \qquad (13)$$

Considering the feed constant (F_A =ct, X_A =ct), from (12) and (13), through linearization can be obtained:

$$sMl\Delta X_B(s) = (-F_{B0})\Delta X_B - F_{D0}\Delta Y_D + (Y_D - Y_{B0})\Delta L(s) - (Y_{D0} - X_{B0})\Delta V(s) \qquad (14)$$

The dependence between mole fraction of the vapour phase ΔY_D (s) and the liquid phase can be expressed using relation (8). Using the relative volatility coefficient α we get:

$$\Delta Y_D(s) = \frac{\alpha}{1 + (\alpha - 1) X_{B0}} \Delta X_B(s) = K(X_{B0}) \Delta X_B(s) \qquad (15)$$

The vapour flow $\Delta V(s)$ is controlled by the heat flow ΔQ_B (s), through the transfer function of the reboiler H_{RB} (s): $\Delta V(s) = H_{RB}(s) \Delta Q_B(s)$ (16)

Using (14), (15) and (16), after several simple transformations, we get:

$$\Delta X_B(s) = \frac{Y_D - X_B}{M_L s + F_{B0} + K F_{D0}} \Delta L(s) + \frac{Y_{D0} - X_{B0}}{M_L s + F_{B0} + K F_{D0}} H_{RB}(s) \Delta Q_B(s) \qquad (17)$$

where F_{B0} and F_{D0} are molar flows. It can be seen in this case, that the system representing the column is stable since $M_L > 0$, $F_{B0} + K F_{D0} > 0$.

Problems can occur in practice since mass flows are measured instead of molar

flows. If the fluid is mono-component there is no problem to convert from molar to mass flow. But usually the fluid in the control flow L is a mix of two components: a high volatile component having a mole fraction y_D and a low volatile component having a mole fraction $(1-y_D)$. The relation that gives the molar mass of the mix is

$$M=Y_D M_1+(1-Y_D)M_2 \text{ [Kg/Kmol]}$$

where M_1 and M_2 are the molar masses of the two components and the mass flow can be determined from the molar flow using relation:

$$L_m=ML=[y_D M_1+(1-Y_D)M_2]L \quad (18)$$

Through linearization of (18) around a steady state value we get:

$$\Delta L_m = [Y_D M_1 + (1-Y_D)M_2]\Delta L + L_0(M_1 - M_2)K(x_{B_0})\Delta X_B \quad (19)$$

Replacing in (14), after several simple transformations we get:

$$\Delta X_B(s) = \frac{Y_D - X_B}{M_0}\cdot\frac{1}{M_L s + a_m}\cdot\Delta L_m(s) + \frac{Y_D - X_B}{M_0}\cdot\frac{1}{M_L s + a_m}\cdot H_{RB}(s)\Delta Q_B \quad (20)$$

where:

$$a_m = F_B + K\cdot F_D - \frac{Y_D - Z_B(M_2 - M_1)}{M_0}\cdot K(x_{B_0})\cdot L_0 \quad (21)$$

It can be seen from relation (21) that there are regions of the operating domain where the system is unstable or at the stability limit ($a_m<=0$). This can be seen also from the static characteristic of the system L [Kmol/min]-Lm [Kg/min] presented in (18), where singular points of the system (of knot, saddle or source type) are present, and function of the sense of variation of the control variable.

4. CONCLUSIONS

The paper presented some practical aspects studied by the authors during experimental research work on the distillation columns at the chemical plant and during the simulation studies.

The results show that, during the implementation of the control structures for industrial installations, maximum care shall be taken for the following:

- sensors selection (characteristics, sensitivity) especially for indirect measurement of the process variables;
- the adequate placement of the sensors in order to measure the useful variations of the parameters, without being affected by the process disturbances;
- the adequate selection of the control variables and sensors-valves pairs;
- the study of the process using real elements that will be used in practice, since internal influences can occur, influencing the effects of the command.

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