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Simulation and Control of Bench-Scale Distillation Columns Using a Switched Reflux Strategy

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The undeniable importance of industrial distillation has motivated hundreds, if not thousands of theoretical and applied research projects. A considerable amount of those projects has used a bench or pilot scale distillation columns to have experimental confirmation of the proposed innovations. Nevertheless, the automatic control of bench scale distillation columns is not as straightforward as it appears to be, due to the low magnitude of the involved material flows. To precisely manipulate low magnitude flows, special low flow control valves are necessary; this results in high instrumentation costs which are not desirable at bench nor pilot scale.

This work treats the simulation and control of a low cost, bench scale column with an electrically heated reboiler and water-cooled condenser. It uses a version of an on-off valve as an actuator to control the distillate composition of the desired product. The use of a solenoid valve results in a discontinuous reflux flow, which changes the continuous dynamical model of the distillation column to a piecewise dynamical one. In other words, it can be assumed that the column switches between zero and infinite reflux ratio instantly. The resulting piecewise dynamic model is studied and analyzed, and because of this analysis, the dynamic implications of this strategy in the operation of the column are used to tune a PID-PWM controller and to formulate general recommendations to attain an efficient composition control in the distillate.

1. Introduction

Academic and industrial bench (or laboratory) and pilot scale experimentation are common in the field of distillation. A wide number of experimental studies have been conducted along the last 2 decades, most of them at bench or pilot plant scale. Studies in the fields of reactive distillation (Pirola et al., 2013), new technologies such as Heat Integrated Distillation Columns (Naito et al., 2000) and Dividing Wall Columns (Dwivedi et al., 2013), process identification (Huyck et al., 2011), process control (Balasubramhanya and Doyle, 2000), and clean fuels (Ceron, 2010). The size of the previously cited column varies from 10-20 plates (Height Equivalent to a Theoretical Plate (HETP) provided by the referenced manufacturer was used were needed).

The scale differences going from 10-50% of the full-scale plant flow don't allow in some cases the use of the same instrumentation and actuators as the full-scale plant, due to costs or availability. Therefore, creative substitutes have to be devised, e.g., the use of electric heaters for the reboiler instead of steam (Huyck et al., 2014) and the use of solenoid valves instead of pneumatic or electro-mechanic valves (Dwivedi et al., 2012).

The implementation of an automatic control scheme under non-conventional actuators has been documented; although, there is a general scarcity of a theoretical background for the identification and tuning of such systems. This work aims to provide a first theoretical approach to the mathematical modelling and control of a switched reflux distillation column, by means of continuous piecewise modelling coupled to Internal Model Control based PID tuning.

2. Distillation column model and dynamic considerations

The dynamic modeling of distillation columns has been widely studied in the literature, one of the simplest yet accurate models is the well-known MESH model (Holland, 1981) where Material and Enthalpy balances, molar fraction summation, and phase equilibrium equations are formulated with the aim of portraying the behavior of

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a real distillation column. Alternatives such as non-equilibrium models are also available (Koijman, 1995), yet it is a more specific approach that requires the calculation of the mass transfer coefficients. Thus, the use of equilibrium models is preferred. Also, packed columns which are more common in bench and pilot scales can be modeled using their HETP. Therefore, this work will take advantage of that equivalence to simplify the modeling.

2.1 The MESH Model

Figure 1 shows the layout of a distillation column and its stage along with the control volumes (A, B, C) used for the material and energy balances. The following assumptions will be used for the modeling of a distillation stage:

- At lower pressures the vapor mass of control volumes A and B is negligible
- The Energy content of the vapor in control volumes A and B is negligible
- The heat of mixing is negligible
- Phase equilibrium is assumed.

The dynamic material and energy balances for a stage j and component i with the assumptions stated above are presented in Eq(1) and the energy balance for the stage assuming C components are presented in Eq(2).

$$\frac{N_{i,j}}{dt} = x_{i,j-1} \cdot L_{j-1} + y_{i,j+1} \cdot V_{j+1} + F_{i,j} - x_{i,j} \cdot L_j - y_{i,j} \cdot V_j$$
(1)

$$\frac{dE_j}{dt} = \left(\sum_{i=1}^{C} y_{i,j+1} \cdot H_{i,j+1}^{V}\right) V_{j+1} + \left(\frac{E_{j-1}}{N_{t,j-1}}\right) L_{j-1} + \sum_{i=1}^{C} H_{i,j}^{F} \cdot F_{i,j} - \left(\sum_{i=1}^{C} y_{i,j} \cdot H_{i,j}^{V}\right) V_j - \left(\frac{E_j}{N_{t,j}}\right) L_j$$
(2)

Where x and y are the molar fractions of liquid and vapor respectively, L, V, and F are the molar flows of liquid, vapor and feed respectively, E is the thermal energy, H is the molar enthalpy, the sub-index j indicates the stage the flow is leaving or the stage of the molar accumulation or fraction, the sub-index i indicates the component of the balance and finally the sub-index t indicates the overall stage.



Figure 1: (a) Stage distillation column (b) Detailed diagram of a stage

The component dynamics of the evaporator and condenser are also neglected. The condenser composition is assumed as the top stage composition, and the reflux is assumed approximately at its boiling point, the reboiler composition is equal to the bottom stage vapor flow. Auxiliary equations such as Eq(3) and Eq(4) show the algebraic restrictions corresponding to phase equilibrium and molar fraction summation.

$$y_{i,j}^{eq} = \frac{\phi(y,T,P) \cdot P}{\gamma(x,T) \cdot P^{sat}}$$
(3)

$$\sum_{i=1}^{C} x_{i,j} = \sum_{i=1}^{C} y_{i,j} = 1$$
(4)

2.2 Aspects of the model

Although the modeling of a column by MESH equations is the same for different scales, the hydraulic behavior of the stages was approximated by linear correlation from the steady-state simulation and assumed a constant liquid hold up in each theoretical stage. An industrial distillation column has a considerable amount of control valves, in the case of the bench scale distillation column there are no control valves, the inlet and bottom flows are manipulated by pumps and manual valves, the condenser cooling liquid flow will be manipulated manually, and the heating in the reboiler will be manipulated using an electrical heater. The differential aspect of the column is the condenser which will not be connected to a reflux drum as in Figure 1 but to a funnel-like solenoid (Figure 2) which will alternately guide the reflux flow back to the column or to an external collector. This difference radically alters the continuous nature of the column to a continuous switched column. This supposes a fundamental model change that is shown in Eq(5) and Eq(6) for the condenser.

$$V_2 - sw \cdot L_1 = 0 \tag{5}$$

$$y_{i,2} \cdot V_2 - x_{i,1} \cdot sw \cdot L_1 = 0$$
(6)

The condenser is counted as the first stage and assumed as a total condenser (Eq(5) and Eq(6)) without accumulation. A new Boolean variable sw is introduced as a switching parameter that changes the operation of the column from total reflux to zero reflux.



Figure 2: New column configuration with reflux funnel solenoid (variable sw)

3. Dynamics of the switched column

The new sw variable introduces an unstable dynamic to the column that compromises the system stability, yet this configuration eliminates the reflux drum accumulation. This means that there are only two accumulations that need to be regulated within the column, the pressure, and the reboiler accumulation. As mentioned before

the condenser duty is such that it will always work as a total condenser; therefore, the water flow to the condenser is fixed such that it can condense vapor flows allowing a permissible range of pressures. The reboiler accumulation can be controlled by the manipulation of the reboiler vapor rate or the outflow pump or valve, one of the scale restrictions is simplicity; therefore, the most practical thing to do will be to manipulate the reboiler duty and in consequence the reboiler vapor flow rate. In this case, a control loop to maintain the reboiler accumulation at a steady value must be implemented. With tight control of the reboiler mass accumulation, it is possible to analyze the dynamics of the column distillate composition as sw is varied.



Figure 3: Step test responses for the binary mixture of methanol and isopropanol a) Step test for sw 0-1 at time 20 min b) Step test for sw 1-0 at time 0.2 min.

Figures 3a and 3b show a 10-stage column response for a binary mixture of methanol and isopropanol, it also shows the different behaviour induced into the column for the switch close (sw 0-1), 20 min after reaching steady state and for the switch opening (sw 1-0) 0.2 min after reaching the steady state, respectively. Figure 3a shows an order one dynamics which transfer function is shown in Eq(7) and, Figure 3b shows an integrating system which transfer function is shown in Eq(8).

y(s) 0.4761	17
$\overline{u(s)} = \frac{1.5936s + 1}{1.5936s + 1}$	(7
y(s) = -0.4787	(0
$\frac{u(s)}{u(s)} = \frac{s}{s}$	(6

4. Distillate molar fraction control

After this step test, it was clear that the closed dynamics was stable and slower than the opened dynamic which was also unstable. Therefore, a PI control was coupled to a Pulse Width Modulator actuator to manipulate the switch variable (sw) to control the distillation molar fraction. In this case for simplicity, it is assumed that it can be measured directly at the distillate output, which is not always possible.

The Pulse Width Modulator (PWM) is often used in power electronics as an actuator in the control of power converters (Angulo et al., 2007) and inverters (Rodriguez et al., 2014). In fact, it is very useful to deal with fast dynamics; nevertheless, the distillation column is not as fast as electronic and electrical systems and presents a slow dynamic switched with a fast dynamic, this makes the selection of the PWM switching frequency one of the most essential tuned parameters.

Preliminary lead to the conclusion that the switching frequency of the PWM must be between 2 times and five times the time constant (τ) of the slow response. In the case of the methanol Isopropanol distillation a switching

frequency of 0.1 Hz. After that, most of the moderate PI controller tunings will work. Nevertheless and due to the simplicity of the IMC-PID tuning rule Eq(9) from Bequette (2003) was used.

$$k_{c} = \frac{\tau_{p}}{k_{p}\lambda}, \ \tau_{I} = \tau_{p}$$
(9)

Where the proportional constant (k) has the sub-index c for the controller and p for the process, τ_I is the controllers integral time, and τ_p is the process time constant.



Figure 4. a) Stabilization response of the controlled system during the start-up b) System response after a 5 % perturbation in the input flow and average (in red)

5. Results

To test the distillation column tuning and response two different scenarios were tested, the first one is the column startup. A simple manual startup strategy was used before turning on the controller. First, the column was stabilized without a continuous feed until it reached a high concentration, after that the nominal feed 1 mol/min started and after 0.5 minutes the controller was turned on (Figure 4a). After the system is oscillating around the setpoint value of $x_D = 0.9$, a 5 % step perturbation is induced on the feed (Figure 4b). For both tests, the average distillate concentration and variance is computed, and the IAE is measured for both test scenarios.

Table 1: Results

Scenario	Average x _D	Variance	IAE
Column Start	0.9002	5.0827E-06	0.0389
Perturbation	0.8997	4.9110E-06	0.0751

Table 1 shows that the average distillate concentration of 0.9002 was achieved after 20 minutes with an acceptable variance, it also indicates that the system rejects perturbations as the average of the distillate composition stabilized at 0.8997 with an acceptable variance. Both responses can be seen in Figure 4 demonstrates that the PID-PWM control strategy is viable for the distillation column start and for perturbance rejection allowing the reduction of costs in bench and laboratory scale columns.

6. Conclusions

The switching frequency of the PWM is the main tuning parameter that allows the PID controller to work correctly, also as a recommendation, non-aggressive PID tunings must be used to allow low variances of the response variable. Although the use of the switched reflux strategy is currently used in laboratory equipment, it is only mentioned briefly in the literature, this works approach explores the discontinuous nature that is inducted on the system by the use of non-conventional actuators, by modelling the system as a piecewise non-linear model with a switching parameter (sw). The achievement of low variances and low IAE Integral index (Table 1), shows that this strategy is effective. The PWM based on the piecewise system identification allowed the identification of the switching frequency of 01 Hz based on the identified slow dynamics, which is used as reference for the control system design.

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