17th European Symposium on Computer Aided Process Engineering – ESCAPE17
V. Plesu and P.S. Agachi (Editors)
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Closed-loop Implementation of Optimal Trajectories in Batch Distillation

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Abstract

In order to implement a quasi-optimal trajectory derived from pinch theory [1,2], a temperature tracking control system composed by an open-loop reflux ratio control plus a closed-loop correction for disturbance rejection is proposed. To adjust the closed-loop controller we use the referential dynamic reaction of the process [3] and tuning rules [4] that, though they were originally developed for dynamics valid in the neighborhood of stationary operating points, under this strategy they are useful in the neighborhood of a reference transient evolution like those occurring in batch distillation columns. The separation of the light component from its ternary mixture of alcohols is studied here.

Keywords: Batch Distillation, Conceptual Model, Process Reaction Method.

1. Conceptual Model

In order to perform a simulation run of a batch rectifier with an infinite number of stages, two design variables have to be selected in addition to the feed composition. We select the distillate composition plus the final rectification advance. Then, the recoveries of the components in the distillate as a function of rectification advance are estimated by integrating the following equations:

$$\frac{d\sigma_i^D}{d\eta} = \frac{x_i^D}{x_i^0}$$

where σ_i^D is the fractional recovery of component i in the distillate, η is the rectification advance, x_i^D is the mole fraction of component i in the distillate, and x_i^0 is the initial mole fraction of component i in the still. The instantaneous minimum reflux ratio R_{min}^{inst} to achieve the pre-fixed distillate composition is estimated from linearization of column profiles at instantaneous still composition x_B, which requires solving an eigenvalue problem of the Jacobian of the equilibrium function in x_B as explained elsewhere [5,6].
The key ingredient of the model is illustrated in Figure 1(a) for the mixture methanol-ethanol-isopropanol. Figure 1(a) shows the mass balance line given by the desired distillate composition x_D (pure methanol), the vapor feed to the rectifier (vapor y_{xB}^* in equilibrium with the instantaneous still composition x_B) and the composition x_N of the liquid leaving the rectifier lower end. The last composition is calculated as the intersection between the mass balance line and the line formed by the two controlling pinch points; i.e; x_B and x_P^{II}. Good agreement between rigorous [7] and simplified simulation [6] is found as shown in Figure 1(a). Figure 1(b) shows the evolution of the minimum reflux ratio necessary to achieve high purity methanol at the top of a column having an infinite number of stages. The still is charged with 90 kmol of a mixture with composition 0.5 methanol, 0.25 ethanol, 0.25 isopropanol and the vapor flow rate V is 30 kmol/h. The predicted recovery of methanol at column top is 94 %.

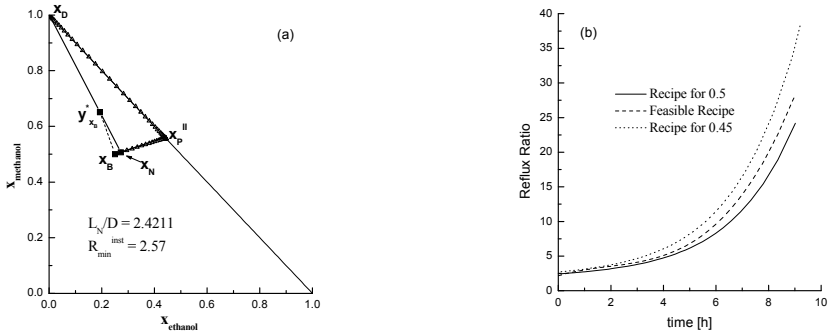

Figure 1(a). System MeOH-EtOH-IPA. (a) Instantaneous minimum reflux (b) reflux ratio versus time.

2. Open-Loop Rigorous Simulation and Tray Temperature Selection

Conceptual models based on pinch analysis provide the quasi-optimal evolution of the reflux ratio for a column with an infinite number of stages, which is a good first approximation to the variable reflux policy to be followed when considering a column with a finite number of trays and holdup as shown in [2]. For this reason, implementation of the nominal recipe must be analyzed in terms of product purity and recovery through rigorous simulation of the process in order to make changes to it, if necessary. Three open-loop simulations of a

column with 30 stages were performed to determine a feasible recipe. Whilst implementation of the nominal recipe ("recipe for 0.5" in Figure 1(b)) produced a low purity distillate in maximum amount [97.16%, 42.3 kmol], the reflux ratio evolution predicted by the conceptual model for composition and holdup in the still corresponding to the end of the start-up phase ("recipe for 0.45" in Figure 1(b)) gives rise to a high purity distillate with minimum amount [99.99%, 35.40 kmol]. In the last case, a pinch at column top is maintained through the whole simulation indicating a waste in energy consumption. A recipe in between was selected because of both its adequate distillate purity and recovery [99.87%, 40.03 kmol]. Figure 2(a) shows the evolution of the light species composition along the column. The behavior of the compositions in Figure 2(a) is in stark contrast to that of the second recipe, where 16 stages form a pinch zone, as already mentioned.

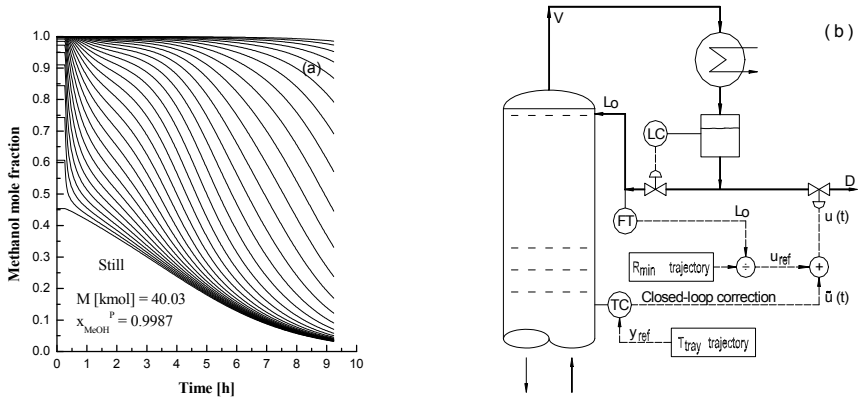

Figure 2. (a) Evolution of the light component composition along the column corresponding to the feasible recipe. (b) Temperature tracking control system formed by an open-loop ratio controller and a referential closed-loop correction.

In order to define a feedback control system, the selection of an appropriate tray temperature evolution (output-reference trajectory) must be done once the feasible recipe is established. The reference trajectory to operate this column is implemented by a simple open-loop ratio controller associated to the condenser-drum level control as shown in Figure 2(b). The distillate flow rate D (input-reference trajectory) has to adapt to the flow measures of the reflux stream L_0, which in turn controls the liquid level in the reflux drum. In this work, the method used to select the reference temperature was to determine the tray temperature that suffers the most important change when the operation goes from total reflux to the final light-component stripping condition. Though alternative techniques can be proposed to select this temperature, the maximum sample variance was successfully used for this purpose. Tray #16 presented the highest value and therefore, the evolution of the temperature at this stage was selected as output-reference trajectory (see Figure 3(b)).

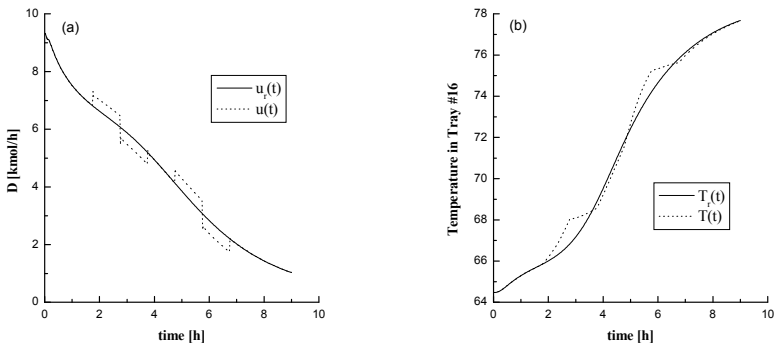

Figure 3. (a) Input-reference and input-perturbed trajectories. (b) Output-reference and output-perturbed trajectories.

3. Referential Process-Reaction Curve and Controller Tuning

The method basically consists of using a standard or nominal time evolution as reference dynamic to determine by contrast the effect of changing the manipulated variable (distillate flow rate) on the controlled one (temperature in Tray #16). Figure 3(a) shows both the input-reference trajectory $u_r(t)$ and the input-perturbed one u(t) made by step changes in the distillate flow rate in such a way that the difference of accumulated amount of distillate is finally compensated. The corresponding output-reference trajectory $T_r(t)$ and the perturbed response T(t) are shown in Figure 3(b). For each input change, a referential process-reaction curve or referential temperature evolution is determined by the difference between the perturbed response T(t) and the reference $T_r(t)$ on the assumption that no other disturbance has occurred. From this curve it is possible to determine the slope, the normalized slope (i.e., slope / input change) and the time delay and therefore, to calculate the parameters for a PI controller using the tuning relations developed by Ziegler and Nichols [4]. Summarizing, the selected controller parameters were: K_c = 0.875 ^oC/kmol and T_I = 1.00 hr.

4. Closed-loop Simulation

In order to show the robustness of the tuning approach, closed-loop simulations were performed for four different cases. Table 1 shows both the initial still composition and holdup for each case. Each still molar holdup was calculated taking into account a constant value for the volume of the vessel. As expected, results of closed-loop simulations of the first cut for cases III and IV did not present any noticeable deviation with respect to the nominal case and therefore, only cases I and II will be analyzed in detail.

Table 1. Compositions and holdup for nominal and perturbed cases.

	Feed Composition	Feed Mole Amount
Nominal Case	**[0.500, 0.250, 0.250]**	**90.00**
Case I	[0.525, 0.250, 0.225]	92.32
Case II	[0.475, 0.250, 0.275]	89.07
Case III	[0.500, 0.275, 0.225]	91.53
Case IV	[0.500, 0.225, 0.275]	89.92

An interesting way to evaluate the performance of the controller is through the analysis of the results of simulations with (closed-loop) and without (open-loop) the tracking of the temperature in tray #16. An open-loop simulation of the mixture corresponding to case I, for example, means the implementation of the nominal feasible recipe by the simple open-loop ratio controller associated to the condenser-drum level control. On the other hand, a closed-loop simulation implies a continuous change in the manipulated variable (distillate flow rate) to track the desired trajectory for the temperature in tray #16. It is clear, from inspection of results in Table 2, that the controller is able to differentiate between separations that are more easier (Case I) and more difficult (Case II) than the nominal case giving rise to high purity products in amounts above (Case I) and below (Case II) the corresponding to the nominal case, respectively.

Figures 4(a) and (b) summarize the results obtained for both cases. The very high purity reported in Table 2 for open-loop operation in case I can be explained by analyzing the behavior of the temperature in tray #16. As shown in Figure 4(a), direct implementation of the nominal recipe gives rise to a temperature evolution that is almost constant with a temperature near the corresponding to pure methanol. This behavior remains for the trays above stage #16 and indicates the existence of a pinch zone, and therefore, a waste of energy. Closed-loop operation, on the other hand, ensures a high purity distillate with increased recovery as a result of a reflux ratio evolution below the nominal as depicted in Figure 4(b). For case II, the temperature evolution for open-loop operation is well above the nominal one. This behavior of the temperature translates into a decrease of product purity with respect to the nominal case. Closed-loop operation prevents such a situation by increasing the reflux ratio above the reference trajectory.

5. Conclusions and Future Work

In this contribution, a novel method is presented that combines the capability of conceptual models based on pinch analysis for predicting the conditions to operate near minimum energy demand, with the simplicity of the referential

reaction method as controller tuning technique to track a desired quasi-optimal temperature trajectory.

The results obtained for the first cut of a ternary mixture of alcohols clearly show the potentiality of the proposed approach and should motivate further research efforts involving problems such as the effect of noise or disturbances in the collected data, or the extension to the whole batch operation including both main and intermediate cuts, with or without a chemical reaction in the still.

Table 2. Performance comparison between simulations for cases I and II, and simulation of the nominal case.

	Product Amount [kmol]	Product Purity [mol %]
Case I – Open loop	40.03	99.989742
Case I – Closed loop	43.78	99.763227
Nominal case	**40.03**	**99.871839**
Case II – Open loop	40.03	97.605938
Case II – Closed loop	37.19	99.913690

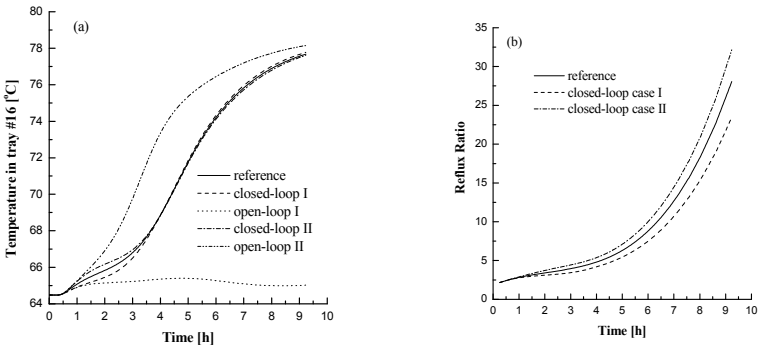

Figure 4. Simulation results (a) Temperature versus time. (b) Reflux ratio versus time.

References

1. J. Espinosa, E. Salomone and O. Iribarren, Ind. Eng. Chem. Res., 43 (2004) 1723.
2. S. Brüggemann, J. Oldenburg, and W. Marquardt, In: FOCAPO 2004, 247.
3. J. L. Marchetti, AIChE J., 50 (2004) 3161.
4. J. G. Ziegler and N. B. Nichols, Trans. ASME, 64 (1942), 759.
5. H. Offers, R. Düssel and J. Stichlmair, Comput. Chem. Eng., 19 (1995) S247.
6. J. Espinosa, and E. Salomone, Ind. Eng. Chem. Res., 38 No. 7 (1999), 2732.
7. Hysys User Manual, 1999, Hyprotech Ltd.: Calgary, Canada.