An Advanced Strategy for Composition Control in Batch Distillation

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Abstract: An advanced strategy for the feedback control of constant-distillate-composition batch distillation is proposed. The control law is derived within a Nonlinear Internal Model Control framework. A closed-loop observer is used to reconstruct the systems states required for the computation of the control action. The proposed controller is easy to tune, and is shown to outperform a conventional PI composition controller significantly. The engineering effort for the development and implementation of the proposed strategy is discussed.

Keywords: Batch distillation, Nonlinear control, Model-based control, Observer

1. INTRODUCTION

The current increasing production of small-volume, high-added-value products has called attention to batch production technologies. Although batch distillation typically consumes more energy than continuous distillation, it provides more flexibility and involves less capital investment. Thus, since energy costs are not too significant in the separation of small-volume, high-added-value products, batch distillation is often attractive to obtain this class of products. Moreover, it is well known that current product market is characterized by a frequently changing demand. A batch column can accommodate this varying demand quite easily, thus tailoring products to customers' needs precisely and timely.

Two basic methods of operating a batch column are usually considered: constant reflux ratio, and constant distillate composition. Optimal-reflux-ratio operation can be viewed as a generalization of constant-reflux-ratio operation, since it often involves a piecewise-constant-reflux-ratio policy, according to a schedule determined by maximizing off-line the desired profit function.

Despite the large number of recently published works on the modeling, simulation, and optimization of batch distillation (Macchietto and Mujtaba, 1996), relatively few papers have addressed the issue of feedback control of a conventional (i.e. rectifying) batch column. Sorensen and Skogestad (1994) and Sorensen *et al.* (1996) considered several strategies for the control of a reactive batch column. Quintero-Marmol *et al.* (1991), and Quintero-Marmol and Luyben (1992), studied the feedback control of a constant-reflux-ratio-operated batch column. Bosley and Edgar (1993) and Macchietto *et al.* (1995) addressed the problem of implementing on-line the optimal operational trajectory determined *a priori* by off-line optimization of the system performance.

This paper is concerned with constant-distillate-composition operation of a batch rectifier. Finefrock *et al.* (1994) pointed out that, since a batch column is an integrating system, the depletion of light components throughout a run creates a control problem somewhat like a ramp load when composition is being controlled. Thus, composition control is very challenging, even for a binary system, because as the reflux ratio increases, the plant gain decreases. If a PI composition controller is employed, the controller gain should be increased during the operation in order to maintain control, and the controller integral time constant should be changed accordingly. The authors suggested using a gain-scheduled PI controller in order to overcome this difficulty. A time-based gain-scheduled control gave good results, but the scheduling was shown heavily dependent upon the composition setpoint and also upon the amount and composition of the feed charge. So, a gain scheduling based on an on-line analysis of some system states was proposed. The scheduling was obtained by reconstructing the plant dynamics off-line by means of linear models. This approach yielded a more flexible controller, which however is expected to work well only in the range were the linear models have been fit to the actual plant response. In addition, the off-line computation of the system dynamic characteristics is quite lengthy.

A strategy based on Nonlinear Model Predictive Control was recognized to be one of the best approaches for distillate composition control (Bosley and Edgar, 1993; Finefrock *et al.*, 1994). However, since this strategy requires to solve on-line an optimization problem, it may result computationally intensive, even with the current availability of computing facilities.

Indeed, recent progress in nonlinear model-based control techniques (Bequette, 1991; Henson and Seborg, 1997) has made the practical applicability of nonlinear controllers a reality. Many of these techniques make use of a nonlinear dynamic process model directly in the control law development phase (which is performed off-line). Thus, not only is the controller action inherently "aware" of the process dynamics, but also the control law calculation is straightforward. These features are very attractive for practical implementation. Henson and Seborg (1997) list a number of simulation and experimental studies on the use of such class of feedback controllers. Quite surprisingly, no applications were found in the field of composition control of batch distillation. The purpose of this paper is to provide a nonlinear model-based technique which can serve as a powerful tool to overcome the inconveniences related to the use of classical control strategies for the composition control of batch distillation.

2. THE PROCESS

The separation of a constant-relative-volatility binary mixture is considered as a test case.

Vapor boilup (V), mol/h	100
Tray holdup (steady state) (H_{i0}), mol	1
Reflux drum holdup (H_D), mol	20
Total feed charge (H_F), mol	400
Nominal feed composition (x_F)	0.5
Estimated feed composition ($\hat{x}_F$)	0.7
Tray hydraulic time constant (β), h	0.001
Number of ideal trays (N)	15
Relative volatility (α)	1.8
Nominal composition setpoint ($x_{D,sp}$)	0.95

Table 1. Process and system characteristics

The process is similar to the one considered by Quintero-Marmol *et al.* (1991). However, differently from that model, the tray hydraulics has been taken into account via a linearized Francis weir formula. The process and system characteristics are summarized in Table 1. In the following, we will refer to this model as to "the plant" or "the process".

3. CONTROL STRATEGIES

3.1 *Conventional approach*

The conventional strategy for constant-composition operation of batch distillation columns usually comprises a total-reflux startup phase, which is carried out until the process approaches steady state. Then, a PI controller is switched on to drive and maintain the distillate composition to the desired value (by manipulating the reflux valve, for example). Finally, the operation is stopped when the reflux ratio reaches a pre-specified limiting value.

3.2 *Proposed approach*

The startup procedure is the same as the one used in the conventional approach. For the development of the proposed control law, a nonlinear model of the process, similar to the one illustrated in the previous Section, is considered. However, in order to account for structural process/model mismatch, the tray hydraulics is neglected here. Thus, the model equations are the same considered by Quintero-Marmol *et al.* (1991), and they will be omitted here for conciseness. The controller model is obtained by recasting the model equations into a state-space notation:

$$\begin{aligned} \dot{\hat{\mathbf{x}}} &= \mathbf{f}(\hat{\mathbf{x}}) + \mathbf{g}(\hat{\mathbf{x}})u \\ \hat{z} &= h(\hat{\mathbf{x}}) \end{aligned} \quad , \qquad (1)$$

where $\mathbf{x}$ is the state vector, $\mathbf{f}(\mathbf{x})$ and $\mathbf{g}(\mathbf{x})$ are vector fields, $u = R$ is the manipulated input (reflux rate), $h(\mathbf{x})$ is a scalar field (the controlled output), and the symbol ^ indicates an estimated property. The controlled variable is the overhead composition, the measure of which is not usually available on-line. In fact, composition analyzers suffers from high investment and maintenance costs; also, they provide delayed measurements, which are not compatible with an effective control, especially in a relatively fast process like a batch distillation. Therefore, the distillate composition must be estimated on-line by using available, low-cost, fast measurements (such as temperatures, for example). We will indicate with $\hat{z} = \hat{x}_D$ the *estimated* distillate composition. The estimation algorithm will be discussed in the next Subsection.

A strategy based on a modified Nonlinear Internal Model Control (NIMC; Henson and Seborg, 1991) will be developed in the following. NIMC belongs to the class of geometric controllers which linearizes the system input-output map exactly. Only the fundamentals of the method will be illustrated here. Some concepts from the differential geometry theory need to be recalled.

The Lie derivative $L_q\lambda(w)$ of the smooth scalar function $\lambda(w)$ with respect to the smooth vector field $q(w)$ is the scalar function defined as:

$$L_q\lambda(w) = \sum_{i=1}^{n} \frac{\partial \lambda(w)}{\partial x_i} q_i(w) \quad , \tag{2}$$

where n is the dimension of the state vector w. Moreover, the symbol $L_q^k\lambda$ indicates the k-time repeated iteration of $L_q\lambda$, that is $L_q^k\lambda = L_q(L_q^{k-1}\lambda)$, with $L_q^0\lambda = \lambda$. Similarly, $L_pL_q\lambda$ is the Lie derivative of $\lambda(x)$ made first in the direction of $q(x)$, and then in the direction of the smooth vector field $p(x)$. The relative order r of a process model like (1) is defined as the least integer for which $L_gL_f^{r-1}h(\hat{x}) \neq 0$. Thus, the relative order of a process model is the number of times that the output must be differentiated with respect to time in order to recover the input u explicitly. Roughly speaking, it is a measure of "how directly" the input affects the controlled output.

Following the above notation, the NIMC control law is the following (Henson and Seborg, 1991):

$$u = \frac{\alpha_1 e - \sum_{k=1}^{r+1} \alpha_k L_f^{k-1} h(\hat{x})}{L_g L_f^{r-1} h(\hat{x})} \quad , \tag{3}$$

with $\alpha_{r+1} = 1$. The error e provides the feedback signal from the plant, and it is defined as $e = z_{sp} - (z - \hat{z})$, where the suffix *sp* refers to the setpoint value. The coefficients α_i are the controller design parameters. Note that no integral action is provided explicitly by this control law. The NIMC technique employs the process model as an open-loop observer, for which observability is not required. It can be proven (Henson and Seborg, 1991) that for open-loop stable, perfectly modeled processes that operate about a stable equilibrium point with $u(t) = u_0$, the model state converges asymptotically to the plant state.

However, a batch column does not operate about an equilibrium point. Moreover, the control objective is to keep the overhead composition x_D close to the setpoint, and this is achieved by continuously varying the manipulated input. Also, a *measure* of x_D is not available. Rather, the distillate composition is estimated by an observer. In this work we employ a closed-loop observer which uses some temperature measurements from the plant in order to improve the estimate of the plant state vector. Therefore, we assume that the controlled output is the *estimated* distillate composition ($\hat{z} = \hat{x}_D$). The NIMC control law will be modified accordingly. In particular, it will be assumed that the model is perfect ($z = \hat{z}$; $e = z_{sp}$). Note that this assumption is reliable only if the observer estimations are good. Under this assumption, the NIMC structure closely resembles the GLC approach of Kravaris and Chung (1987).

It can be shown that the relative order of model (1) is $r = 2$. In practice, this is because total condensation of the overhead vapor is assumed ($g_D(x) = 0$), so that the reflux can affect the distillate composition only through a change in the overhead vapor composition. If the controller tuning parameters are chosen such that $\alpha_1 = \varepsilon^{-2}$ and $\alpha_2 = 2\varepsilon^{-1}$ (where ε is the closed-loop time constant), the resulting control law becomes the following:

$$R = \left[\frac{V(\hat{x}_D - \hat{x}_N)}{H_D H_i}\frac{\partial \hat{y}_N}{\partial \hat{x}_N}\right]^{-1}\left\{\frac{x_{D,sp} - \hat{x}_D}{\varepsilon^2} - \frac{2V(\hat{y}_N - \hat{x}_D)}{\varepsilon H_D} - \frac{V}{H_D}\left[\frac{V}{H_i}(\hat{y}_{N-1} - \hat{y}_N)\frac{\partial \hat{y}_N}{\partial \hat{x}_N} - \frac{V}{H_D}(\hat{y}_N - \hat{x}_D)\right]\right\} \tag{4}$$

With a perfect process model, and a system that is initially at rest and with $z(0) = z_{sp}(0)$, the system closed loop transfer function for setpoint changes is:

$$\frac{Z(s)}{Z_{sp}(s)} = \frac{1}{(\varepsilon s + 1)^2} \quad . \tag{5}$$

Equation (5) provides a way to tune the controller. Following the classical startup procedure, the column can be operated at total reflux until steady state is approached. Then, the NIMC controller is switched on, and the tuning parameter ε is adjusted until the desired plant speed of response is achieved. By proceeding in this way, under the limiting hypothesis that the process state was perfectly known at any time, the closed-loop time constant was set to $\varepsilon = 0.1$ h. This value was retained in all the simulations presented in this work. In order to avoid excessive spikes on the reflux rate (which are not advisable in an actual plant), the reflux profile was passed through a rate-of-change filter (Seborg *et al.*, 1989). Alternatively, one could consider filtering the setpoint, as indicated by Henson and Seborg (1991).

3.3 *State estimation*

In order to apply the control law (4) successfully, some of the column states must be estimated. For a binary system, the tray compositions could be estimated directly by static temperature measurements; however, this is not possible for the distillate composition. In this work, we take a more general approach, which can be used also for multicomponent mixtures and with a limited number of available temperature measurements. If the system is observable, a closed-loop observer can be implemented in order to reconstruct the system states. By applying a degree-of-freedom analysis, Yu and Luyben (1987) showed that a Nc-component *continuous* distillation column is observable about the operating point as long as at least $Nc-1$ temperature measurements are available. The task of proving the observability of a *batch* column is not trivial, since the column does not operate about a steady state. Linearization about the column nominal *trajectory* gives rise to a time-varying system, whose observability cannot be proven unless the observability Gramian matrix is calculated (Ray, 1981). For the system considered, this is impossible to do analytically.

However, differential geometry provides a powerful tool for a rigorous evaluation of local observability of nonlinear systems. The model considered in the previous Subsection is now recast into:

$$\begin{aligned} \dot{\hat{\mathbf{x}}}(t) &= \mathbf{r}(\hat{\mathbf{x}},\mathbf{v},t) \\ \mathbf{T}(t) &= \mathbf{g}(\hat{\mathbf{x}},t) \end{aligned} \qquad (6)$$

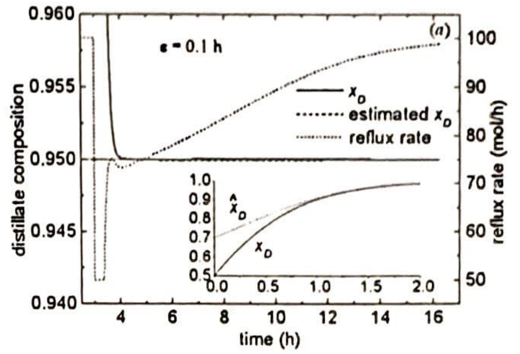
where $\mathbf{v}$ is now the vector of the system input (R) and measurable disturbance (V), and $\mathbf{T}$ is the vector of plant measurements (temperatures). In order to assess the system observability, we will assume that a single temperature measurement is available from the plant (thus, $\mathbf{T}$ is a scalar, which depends on a single state). Following Muske and Edgar (1997), if the observability matrix -- made up of the row vectors of $\{L_r^{j-1}(\mathrm{d}g),\ \ j=1,2,\ldots,N+3\}$ -- has full rank along the nominal trajectory, then the system is locally weakly observable. After some cumbersome computations, it can be shown that the elements of the observability matrix can be computed analytically. The observability matrix results in a very complex function of all states. Its structure is compatible with the full-rank condition, regardless of the location of the temperature measurement. Thus, the system may well be locally weakly observable.

The observer used in this paper is the extended Luenberger observer proposed by Quintero-Marmol *et al.* (1991). For the sake of conciseness, the observer design procedure will not be recalled here. Note that in all the simulations we have actually used two temperature measurements (namely T_B and T_{10}) as feedback signals from the plant.

It should be remembered that batch columns are often operated through chains of operations, which may involve the mixing of fresh feed with recycled cuts. Thus, a major source of process/model mismatch is the lack of precise knowledge of the feed composition. Thus, if the observer dynamics is not designed so fast for the observer as to reconstruct the system states quickly and precisely, the model-based controller performance may be severely degraded, since no explicit integral action is provided by the NIMC control law previously derived.

4. RESULTS AND DISCUSSION

The sampling/control interval was set to $\Delta t = 0.01$ h in all the runs presented in this work. The performance of the control law (4), when the error in the feed composition estimation is quite large ($\hat{x}_F = 0.7$), is shown in Fig. 1*a*. Although the estimation of x_D is not good at the very beginning of the operation (see detail in Fig. 1*a*), it improves very rapidly, in such a way that the model-based controller action is very effective.



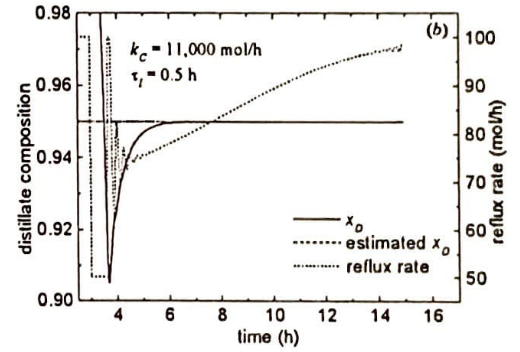


Fig. 1. Plant response to the (*a*) NIMC and (*b*) PI controllers under nominal operation. A detail of the observer performance at the beginning of the operation is magnified in (*a*)

As for the PI controller, some time was needed to get a satisfactory tuning. Finally, the controller performance was acceptable (Fig. 1*b*), although it should be noted that during the transition from the startup to the production phases the distillate composition undershoots the setpoint significantly, and some oscillations in the manipulated variable are noticed.

By retaining the controller settings used in Fig. 1, the controller performances were evaluated at operating conditions other than the nominal ones. For example, a feed richer in the heavy component was charged to the plant ($x_F = 0.3$), and the distillate composition setpoint was increased ($x_{D,sp} = 0.985$). The NIMC controller performance (Fig. 2*a*) remained very good. As expected, the plant response to the PI controller was instead severely degraded (Fig. 2*b*). In fact, due to the presence of the model terms in the control law (4), the nonlinear controller continuously updates the control action strength according to the varying system dynamics. Conversely, the aggressiveness of the PI controller action cannot be modified in the face of the new dynamic behavior of the system.

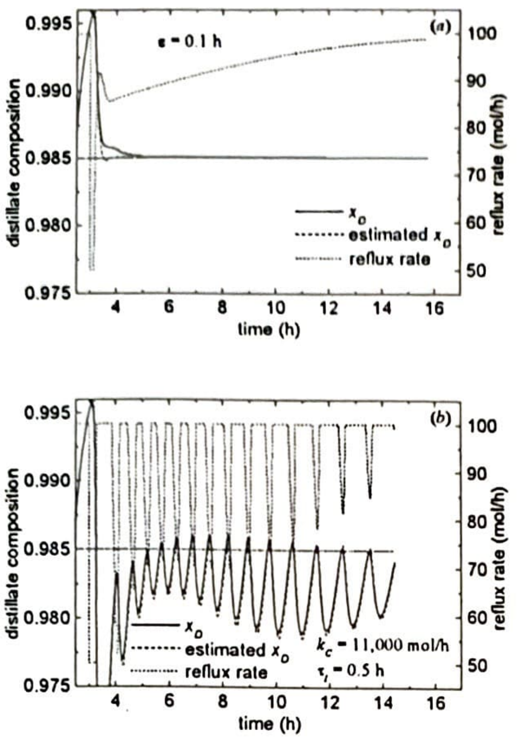


Fig. 2. Plant response to the (*a*) NIMC and (*b*) PI controllers under operating conditions different from the nominal ones ($x_F = 0.3$, $x_{D,sp} = 0.985$)

It is interesting to point out that, compared to operation at constant reflux ratio, larger errors in the estimated feed composition can be accommodated by the observer. This is due to the fact that, while approaching the steady state, the dynamics of the column is somewhat "freezed", in such a way that the observer has enough time to accurately reconstruct the system state vector. Thus, regardless of the controller used, the conventional startup strategy results advantageous from the point of view of the state estimation.

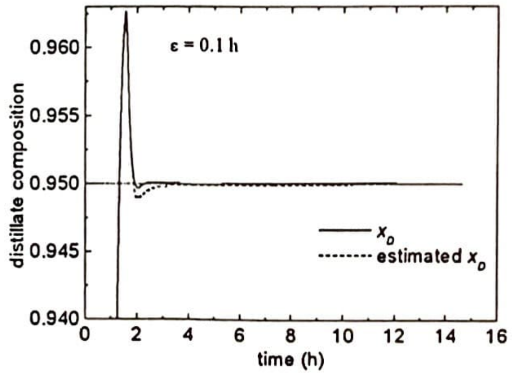


Fig. 3. Performance of the NIMC controller in the case of a modified startup policy

However, approaching the steady state may be time consuming. For this reason, the possibility of switching on the NIMC controller as soon as the estimated distillate composition reaches the setpoint was investigated. It can be seen from Fig. 3 that the nonlinear controller performed very well. Although the state estimation may not be very good at the beginning of the operation, the control law captures the main dynamic features of the process with good accuracy, and the distillate composition is driven to the setpoint quickly.

It is well known that the Luenberger observer is a deterministic estimator. Although the problem in chemical processing is more often the lack of measurements than the low quality of measurements (Wallman, 1979), one should be aware that the observer may not work properly when the available measurements are corrupted by noise. Usually, temperature measurements are not affected by noise very heavily. Noise spikes can be easily filtered out, but a background noise may well be present. The presence of this kind of noise was simulated by adding zero-mean random numbers with a standard deviation of $\sigma = 0.1\,°C$ to the temperature "measurements".

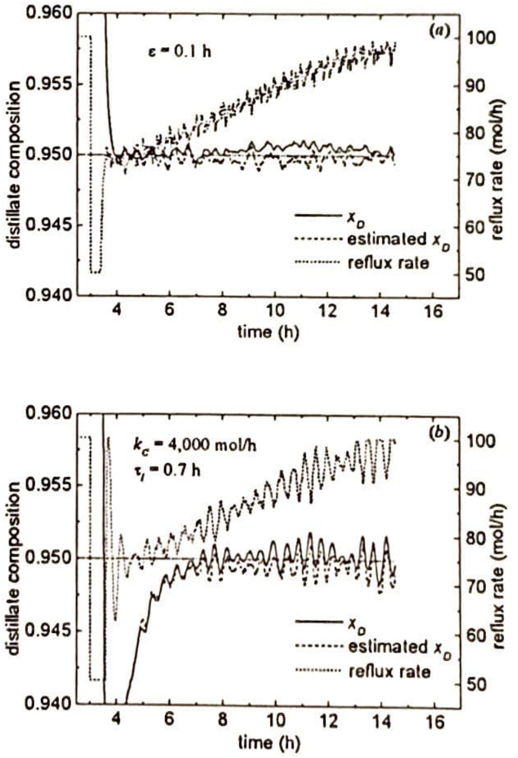


Fig. 4. Plant response to the (*a*) NIMC and (*b*) PI controllers under nominal operation and noise on the temperature measurements

The nonlinear controller performance is still satisfactory (Fig. 4*a*). This is due to the inherent robustness of the Luenberger observer. However, if a large degree of noise is expected, the use of a probabilistic estimator (like a Kalman filter) would be advisable. The PI controller with the previously determined tuning pushed the process towards instability. Though the controller was detuned, its performance still appeared to be somewhat compromised (Fig. 4*b*).

5. CONCLUSIONS

An advanced strategy for composition control in batch distillation operations has been proposed. The control law has been derived within a NIMC framework. State estimation, which is necessary for the practical implementation of the proposed control law, has been provided by an extended Luenberger observer. The proposed approach has been shown to outperform a conventional PI strategy by a great deal. The controller performance is not affected by changes in the feed composition or in the composition specification. The engineering effort for the development and implementation of the proposed approach can be summarized as follows. *i)*. The control law development is not trivial, but it can be carried out off-line in a very general way (i.e. it does not depend either on the system or on the specification). *ii)*. The control law tuning is very easy, since a single tuning parameter needs to be adjusted for satisfactory performance. In addition, the tuning appears to be independent of the operating conditions. *iii)*. By following the guidelines provided by Quintero-Marmol *et al.* (1991), the extended Luenberger observer design can be carried out quite easily. *iv)*. The computation of the control law is straightforward, which is an important feature for on-line application. The major computational burden is related to the state estimation, that is to plant simulation through a model running in parallel to the plant. However, since no optimizations are required on-line, the required computation time is significantly limited.

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