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Optimal Operation of a Distillation Process Through Extremum Seeking Control

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Abstract: In this work, extremum seeking control (ESC) is applied to optimize the operating conditions of a distillation column in continuous operation, to separate the components of an ideal binary mixture. The approach is based on an objective function that requires both the compositions of the distillate stream and bottom stream in an equal distance from complete purity. Numerical simulations show how the ESC drives the process to the minimum of the objective function, which is typically determined through the construction of a response surface of the objective function with respect to the process inputs. The performance of the standard ESC is compared with an accelerated version including a proportional action.

Keywords: Extremum seeking control, distillate plate column, real time optimization, process control.

1. INTRODUCTION

Distillation in a tray column is the most popular separation process in industry, but also the most energy consuming. Its design and control are therefore aimed at guaranteeing minimal energy consumption while reaching the targeted compositions in their output streams. These systems are modelled by numerous differential equations, where the influences of diverse factors are described by nonlinear relationships (mainly from physical chemistry and thermodynamics), making model-based tasks of design, optimization, and control complex and challenging.

Nowadays, the design of the distillation column operating conditions is carried out in a model-based optimization framework, where either analytical (e.g., Javaloyes-Antón et al., 2022; López-Arenas et al., 2019), stochastic (e.g., Wang et al., 2020) or response surface type (e.g., Vazquez-Castillo et al., 2015) techniques are applied. Any optimization approach requires an extensive computational effort to repeatedly solve the model equations. This computational load depends on the system complexity defined by the characteristics of the mixture and the process equipment. Although recent optimization approaches allow reducing the number of iterations, the system high dimensionality and the impossibility to guarantee the convergence towards the optimum are still limiting factors.

The design of a distillation process includes two complementary aspects: (1) the selection of the process equipment, and (2) the definition of the process conditions. Once the initial design has been achieved, fine tuning is inevitably needed to correct the design errors inherent to modelling mismatches and changes in exogenous factors that affect the process (for instance, the feed stream can evolve over the process lifetime). This process tuning can be carried out through feedback control, which is often relying on conventional PI controllers, whose performance will usually be satisfactory in a narrow operating range. In the early work of Sawaragi et al. (1971), an adaptive method is proposed, using transient measurements to update the input through a trial process. Inspired by the seminal steady-state self-optimizing control framework of Skogestad (2000), Torgashow et al. (2004) have proposed a real-time optimization of the distillation process by sliding-mode control, however requiring a specific set of parameter values to ensure sliding-mode conditions.

In line with such direct input adaptation algorithms, Extremum Seeking Control (ESC, Krstic and Wang, 2000, Ariyur and Krstic 2003) constitutes a promising alternative candidate to achieve process optimization without requiring a full model. ESC indeed estimates in real-time the gradient of a measurable convex objective function (while, in Sawaragi et al. (1971), the decision relies on a logic map), provided that the system is excited by a well-designed periodic dither signal.

This work proposes an exploration of the application of ESC to the distillation column process to design the process in a model lack scenario, which eventually aims to the on-line optimal design and control of this kind of processes. The specificities of the distillation process are presented in Section 2, also describing the model. In Section 3, a reference design of the distillation process is carried out through a response surface technique and the ESC approach is presented in Section 4. The validation of the proposed ESC strategy is achieved considering three optimization scenarios. Conclusions are drawn in Section 6.

2. THE DISTILLATION COLUMN

A distillation tray column in continuous operation is considered (Fig. 1), with n plates, where an ideal-type binary mixture is separated. A thermally conditioned mixture is fed into the intermediate plate n_F, with a composition z and a flowrate F. The term "composition" refers to the mole fraction of the light component in the mixture. The process objective aims at achieving a high composition x_D of the distillate stream (at the column top), while maintaining the bottom stream x_B at low level; in this way, the recovery of the light component in the distillate stream, as well as the one of the heavy one in the bottom stream, is high. The distillation process can be driven by the reflux flowrate (R) and the reboiler duty (Q_R), according to the values of z and F.

The separation process is carried out along the column where the perforated plates enable the descending liquid to reside for a lapse of time and be in contact with the ascending vapor. The vapor and liquid tend to establish a thermodynamical equilibrium, along which the light component in the liquid phase transfers to the vapor phase. Hence, the composition x_i of the liquid, as well as of the vapor y_i, changes from plate i to plate $i-1$, and from plate i to plate $i+1$, respectively; thus, carrying out the separation process.

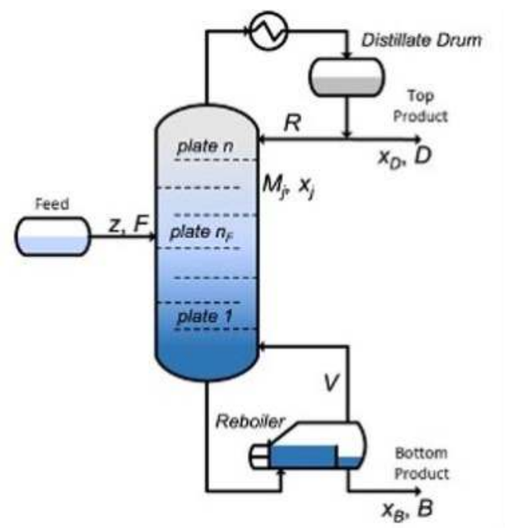

Fig. 1. Continuous distillation tray column

2.1 Mathematical Model

The mathematical model of the distillation column is obtained from material balance and the thermodynamical vapor-liquid equilibrium. The model takes the following form (adapted from Luyben (1996)),

$$\dot{x}_B = \frac{L_1(M_1)}{M_B}(x_1 - x_B) - \frac{V}{M_B}(y_B(x_B) - x_B), \tag{1a}$$

$$\dot{x}_i = \frac{L_{i+1}(M_{i+1})}{M_i}(x_{i+1} - x_i) - \frac{V}{M_i}\big(y_{i-1}(x_{i-1}) - y_i(x_i)\big) + X_i,$$

$$X_i = 0 \text{ if } i \neq n_F,\ X_{n_F} = \frac{F}{M_{n_F}}(z - x_{n_F}), \tag{1b}$$

$$\dot{x}_D = \frac{V}{M_D}(x_1 - x_B) - \frac{V}{M_B}(y_B(x_B) - x_B), \tag{1c}$$

$$\dot{M}_B = L_1(M_1) - B - V = 0$$

$$=> \ B = L_1(M_1) - V, \tag{1d}$$

$$\dot{M}_i = L_{i+1}(M_{i+1}) - L_i(M_i) + S_i,$$

$$S_i = 0 \text{ if } i \neq n_F,\ S_{n_F} = F \tag{1e}$$

$$\dot{M}_D = V - D - R = 0$$

$$=> \ D = V - R \tag{1f}$$

$$y_i(x_i) = \frac{\alpha x_i}{1+(\alpha-1)x_i},\ L_i(M_i) = \bar{L}_i + \frac{M_i - \bar{M}_i}{\beta}, i = 1, \dots, n \tag{1g}$$

where x_B, x_i, and x_D are the compositions of the liquid mixture in the reboiler (located at the column bottom), in the plate i, and in the distillate drum (located at the column top), respectively. y refers to the vapor composition. M_B, M_i, and M_D are the mol of the liquid mixture in the reboiler, in the plate i, and in the distillate drum, respectively. $\bar{M}$ refers to the nominal values. B and D are the flowrates of the bottom stream and distillate, respectively. V is the flowrate of vapor provided by the reboiler, and R is the reflux flowrate at the column top. α is the relative volatility of the mixture, and β is the hydraulics time constant of plate.

This model also assumes that:

- The temperature is constant along the column.
- V is proportional to the reboiler duty (Q_R), $V = kQ_R$, thus V encloses the effect of Q_R.
- The flow of liquid going down (L) from tray to tray is constant, and the flow of vapor going up (V) as well.

The vector representation reads:

$$\dot{x} = f(x, u, d),\ \ x(0) = x_0; \tag{2a}$$

$$x = [x_B, x_1, x_2, \dots, x_n, x_D, M_B, M, M_2, \dots, M_n, M_D]', \tag{2b}$$

$$u = [R, V]',\ \ d = [z, F]' \tag{2c}$$

which is a high-dimensional system ($\dim(x) = 2n + 4$), with two available control inputs (u) and two disturbances (d). $f(\cdot)$ represent the right-hand side functions of the ordinary differential equations that form the process model (1).

System (2a) presents a stable steady state ($x°$) for any feasible operation condition ($u°, d°$),

$$\{f(x, u°, d°) = 0 \Longrightarrow x° = f^{-1}(u°, d°)\}$$

$$\Longrightarrow f(x°, u°, d°) = 0 \tag{3a}$$

$$x(t) = \phi(t, x_0, u°, d°) \Longrightarrow x(t \to \infty) \to x° \tag{3b}$$

The steady state $x°$, given $u°$ and $d°$, means the solution of the $2n + 4$ algebraic equations (3a). The steady state is typically unique and stable, although there exist specific conditions where more than one steady state appear, and at least one of them is unstable (Jacobsen and Skogestad, 1996). In this work, single and stable steady state process conditions are assumed in such a way that every trajectory $x(t)$ tends to $x°$.

2.1 The Design Problem

The starting point considers a distillation column already constructed (i.e., $n = \bar{n}$, $n_F = \bar{n}_F$, and $M_B = \bar{M}_B$, $M_i = \bar{M}_i$, $M_D = \bar{M}_D$ are provided, and β is known), and used to separate a specific mixture (i.e., $z = \bar{z}$ and $F = \bar{F}$ are provided, and α is known). Thus, the problem of the process design consists in determining the operation conditions ($u = u^* =?$) to obtain the maximum composition in the distillate stream ($x_D = x_D^*$), and at the same time the minimum composition in the bottom stream ($x_B = x_B^*$).

In an optimization framework the problem is established as:

$$\min_{(R,\ V)} J = (1 - x_D - x_B)^2 \qquad (4a)$$

$$s.t.\ f(x, u, d) = 0 \qquad (4b)$$

As already mentioned, high x_D and low x_B values imply a high recovery of both components; the light one in the distillate stream, and the heavy one at the bottom stream.

3. PROCESS DESIGN THROUGH RESPONSE SURFACES

In this section, as a reference to validate the results of our ESC approach, the simplest conventional approach is followed, in which there is guarantee that the minimum point of the objective function J (4a) can be located. This approach consists of constructing the response surfaces of x_D and x_B with respect to R and V; next, based on these response surfaces, constructing the response surface of the objective function J (4a), and finally locating the minimum point of J. This implies numerous runs of solving the algebraic equations set (3a) for the points $u°$ on a grid in a $R \times V$-space defined by the feasible values R and V.

To get a reference, the case study from Luyben (1996) is considered with distillation characteristics and process parameters provided in Table 1.

Table 1. Distillation Column Specifics and Process Parameters

Distillation Column		*Binary Mixture*	
n	20	z (%mol)	50
n_F	10	F (mol/h)	100
$\bar{M}_B$ (mol)	100	α	2.0
$\bar{M}_D$ (mol)	100	Constraints	
$\bar{M}_i$ (mol)	10	R (mol/h)	[120, 135]
β	0.1	V (mol/h)	[170, 185]

This system refers to a binary mixture with a medium difficulty of separation (as higher α, the easier the separation), and a column with enough separation steps to obtain output streams with high component of interest even if still not pure.

Fig. 2 depicts the corresponding response surface of x_D and x_B, neither of which exhibits an extremum point, in such a way the location of an optimal operating point ($\bar{R}$, $\bar{V}$) is kind of fussy since a high composition in the distillate likely implies a high composition in the bottom stream; so, if the process design were to be based on these surfaces, the choice of process conditions would be elaborate.

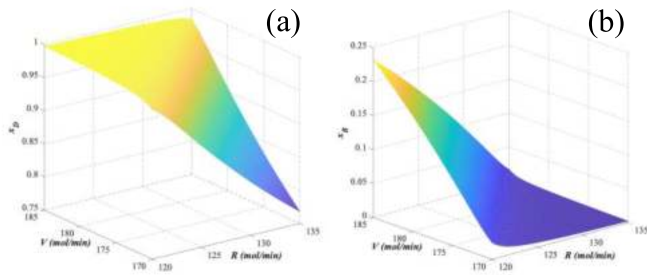

Fig. 2. Response surfaces of light component composition in the (a) distillate stream, and (b) the bottom stream

Fig. 3 illustrates the resulting response surface of J (4a). This surface seems not to have an extremum point, but a channel of points where for every fixed $\check{V}$, there is a $\check{R}$ where J is minimum ($\check{J}$), and vice versa for every fixed $\check{R}$. Although imperceptible at sight, since the channel seems slightly leaned, at $\bar{V}$ = 178 mol/h and $\bar{R}$ = 128 mol/h, J gets its minimum value, which in turn results in $\bar{x}_D$= 0.98 and $\bar{x}_B$= 0.02. This point coincides with the one considered as nominal condition in Luyben (1996).

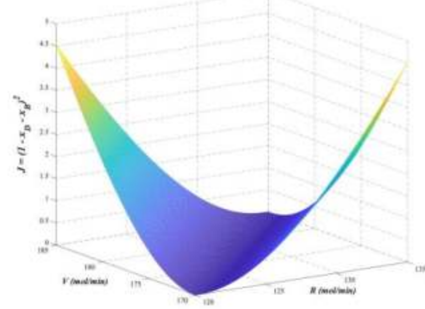

Fig. 3. Response surface of the Objective Function J (4a)

4. OPTIMAL OPERATING CONDITIONS THROUGH EXTREMUM SEEKING CONTROL

In this work we address the design problem through ESC, which is a direct input adaptation estimating the gradient of a supposed static, convex and measurable objective function, to reach its extremum. The estimation of this extremum therefore does not require the full knowledge of the process model and, furthermore, for the purpose of this work, it avoids solving a high dimensional algebraic system, which is an inherent task in any optimal approach of distillation column process design.

An earlier formulation of model-free ESC is proposed in Krstic and Wang (2000) and Ariyur and Krstic (2003) using a bank of filters shown in Fig. 4. The corresponding equations read:

$$\dot{\eta} = -\omega_\eta \eta + \omega_\eta y \qquad \text{where } y = J \text{ (Eq. 4a)} \tag{5a}$$

$$G = (y - \eta)M(t) \tag{5b}$$

$$\dot{\hat{u}} = -K_I G \qquad \text{where } u = R \text{ } or \text{ } V \tag{5c}$$

$$u = \hat{u} + S(t) \qquad \text{where } S(t) = Asin(\omega t) \tag{5d}$$

where $\hat{u}$ and u are, respectively, the estimated and system applied inputs. The latter results from perturbing $\hat{u}$ by the dither signal $S(t)$ (5d); next, the output $y = J$ is passed by a high-pass filter (5a), whose output η yields the gradient estimate G through a demodulation (5b) by $M(t)$ (with the same frequency as $S(t)$ but possibly different phase and magnitudes). Finally, G will drive $\hat{u}$ by an integral-like action (5c). The integral gain K_I, and the amplitude A and frequency ω of $S(t)$ are the tuning parameters.

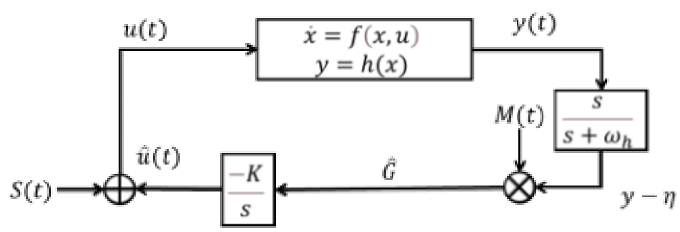

Fig. 4. Classical perturbation-based extremum seeking scheme

The exponential convergence of the algorithm is ensured to an $O(\omega + A)$ neighborhood of the output y if the following assumptions are satisfied:

- The system can be driven to a specific equilibrium represented by a smooth function of the input.
- This equilibrium y_e is locally exponentially stable uniformly on the input u_e.
- The smooth equilibrium (static) function presents a maximum (minimum in our case) for an optimal u_e^* such that:

$$\frac{\partial y_e}{\partial u_e} = 0, \quad \frac{\partial^2 y_e}{\partial {u_e}^2} < 0$$

Although the purpose of this work is on process design by applying a control technique, it is worthy to mention that the application of ESC to relatively slow processes may however present some drawbacks for control purposes since the bank of filters impose a three time-scale separation of, by decreasing order of speed, the process, the estimator, and controller (Dewasme et al., 2017).

Among the several strategies proposed in the last decade, the proportional-integral formulation from Guay (2016) has allowed to significantly accelerate the convergence of the ESC for a class of minimum phase nonlinear systems. This strategy has also provided satisfactory results when extended to bioprocess applications (Dewasme and Vande Wouwer, 2020). In this new configuration, the input is additionally G-driven by a proportional action, and Eq. (5d) is simply replaced by:

$$u = \hat{u} - K_P G + S(t) \tag{6}$$

K_P is the proportional gain.

The new scheme is shown in Fig. 5.

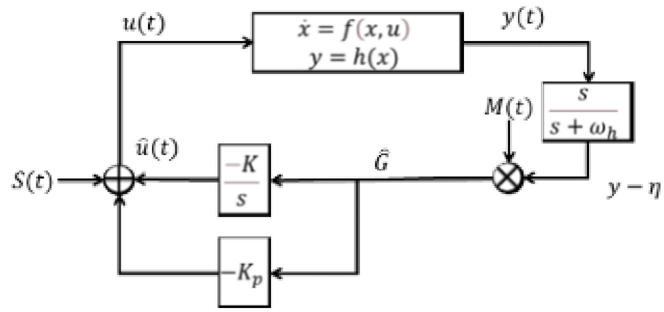

Fig. 5. Proportional-Integral perturbation-based extremum seeking scheme

A comparison of these strategies applied to the distillation process is illustrated in the next section, highlighting the behaviour of the classical ESC and the PIESC and constituting an early single input-single output (SISO) application of ESC to the distillation column. The corresponding optimization problem therefore reads:

$$\min_{(R \text{ } at \text{ } \bar{V})} J = (1 - x_D - x_B)^2 \tag{7a}$$

$$s.t. \text{ } f(x, u, d) = 0 \tag{7b}$$

5. RESULTS

To test and illustrate the two versions of the ESC approach, it is recalled the case study from Luyben (1996) and described in Section 3. It is fixed V at $\bar{V} = 178 \text{ } mol/h$, and in addition to the scenario of separating a mixture with $z = 0.50$, two other mixtures are considered: with $z = 0.45$, and $z = 0.55$. In Table 2, the process conditions where J (4a) takes a minimum value for a feeding mixture of these different composition (z) are given.

Table 2. Optimal process conditions for feed mixtures of different compositions

@ V =178 mol/h			
z	R (mol/h)	x_D	x_B
0.45	133.2	0.9821	0.1811
0.50	128.0	0.9800	0.0200
0.55	122.8	0.9782	0.0223

5.1 Optimal Process Conditions Through Extremum Seeking Control

The following Fig. 6 illustrates the performance of both ESC versions, for a feeding mixture whose composition is $z = 0.50$ (see Table 2).

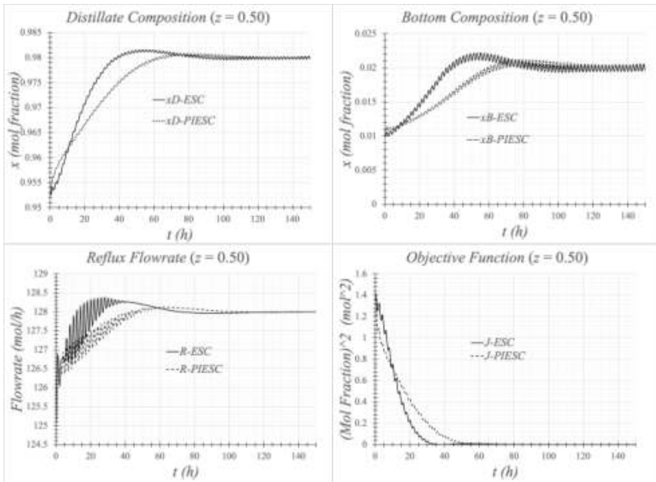

Fig. 6. Seeking of the extremum process condition for a feeding mixture of z = 0.50 at $\overline{\mathrm{V}}$ = 178 mol/h

It can be noticed that the final values of x_D and x_B oscillates around the corresponding optimal values given in Table 2, as well as R, meaning that both versions of the ESC (5, 6) can set the optimal process condition (R^*). Contrary to the expected, the PIESC seems to provide a slower convergence, but it provides smoother trajectories and damped in comparison with the conventional ESC.

In other hand, this process exhibits a natural settling time around 60 h, and the ESC trajectories settles down around 100 h. The oscillatory trajectories that are required to the control input (R) seems to be impractical. These two issues represent disadvantages on using ESC as a process controller in practice.

The tuning parameters of the ESC and PIESC used are:

$A = 3$, $\omega = 2\pi$, $\omega_h = 0.2\pi$, $K = 2$, $K_I = 5$, and $M(t) = S(t)$.

These parameters were also applied to seek the process condition when a mixture of $z = 0.45$ (Fig. 7), and $z = 0.55$ (Fig. 8) is fed to the distillation column. In the comparison of the two ESC versions, the PIESC is not faster than the conventional ESC, as it was expected, but its trajectories are smoother and damped again.

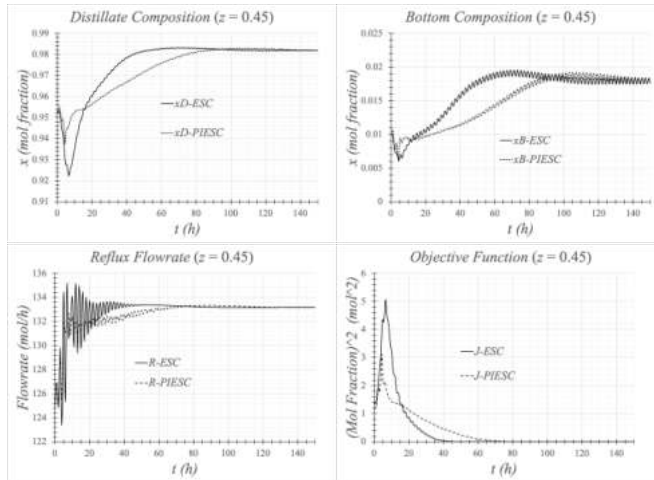

Fig. 7. Seeking of the extremum process condition for a feeding mixture of z = 0.45 at $\overline{\mathrm{V}}$ = 178 mol/h

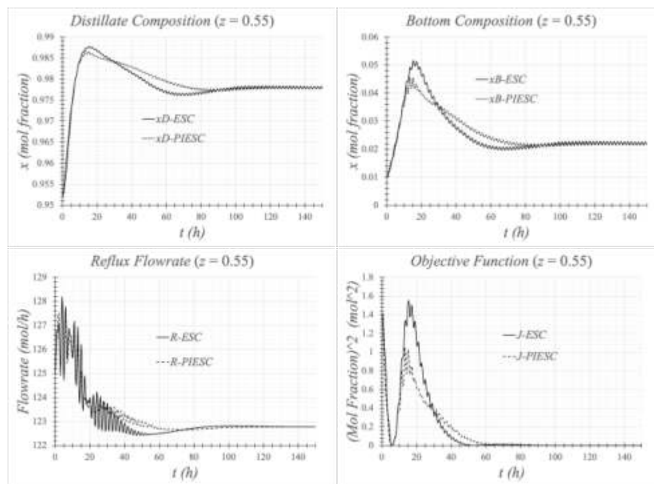

Fig. 8. Seeking of the extremum process condition for a feeding mixture of z = 0.55 at $\overline{\mathrm{V}}$ = 178 mol/h

6. CONCLUSIONS

In this work, optimal process conditions through Extremum Seeking Control were reached for a distillation column in a continuous operation in which an ideal binary mixture is separated. Up to the knowledge of the authors, this is a first work in which ESC is applied to this kind of processes; in this case, it was explored the driving of two process outputs, enclosed in an objective function considered as the output for the ESC technique, by only one control input. Although convergence time is the main disadvantage of the ESC, the outcomes motivate further study on the implications of the ESC to regulate this kind of processes, and even more on designing schemes to use simultaneously the multiple control inputs that are available.

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