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Experimental validation of a high-gain observer for composition estimation in an ethanol–water distillation column

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ABSTRACT: In this paper a high-gain observer used to estimate the product compositions in a distillation column for a non-ideal mixture (ethanol–water) through the tray temperature measurements is presented. The design of this observer is based on a simplified mathematical model. One of the main advantages of this observer is its constant gain, therefore its tuning depends only on choosing a few constant parameters satisfying some simple algebraic inequalities. The effectiveness of the proposed method is demonstrated through on-line experiments in a distillation pilot plant.

KEYWORDS: nonlinear systems; distillation columns; high-gain observer

INTRODUCTION

For chemical processes, the on-line measurement of the variables that are not accessible or that can be measured only as a combination of some state variables is a fundamental difficulty in process engineering. Their main control problems are caused due to tight interactions between the process variables, nonlinearities of the process, process and measurement delays and the large number of involved variables.

State observers, which are generally named ‘virtual or software sensors’, are applied in order to cope with problems associated to the lack of on-line sensors by using on-line and/or off-line measurements (see e.g. Ref.^[1–4]).

In chemical processes, observers have represented a suitable solution to estimate the unmeasured variables despite process disturbances and model uncertainties.^[5,6] Authors in Ref.^[7] developed a state estimator which is stable for systems with probabilistic sensor gain reductions, unknown external disturbance and delayed data.

Distillation is the preferred separation process of fluid mixtures in chemical industry. For this reason,

many research works are in progress in this field (see e.g. Ref.^[8–10]). This work focuses on the estimation problem in distillation columns which is motivated by the necessity of improving their monitoring and control schemes. One important variable to estimate in order to control distillation columns is the product composition.

In order to reconstruct the product composition dynamics some secondary measurements are used (e.g. temperatures and pressures). Therefore a significant amount of effort has been devoted to develop algorithms that provide an accurate parameter identification and state estimation (state observers) in order to perform this reconstruction using secondary measurements (e.g., temperatures and flows).^[11–17]

However, an important difficulty when applying state observers to nonlinear systems is related to the complex calculation of the observer gain, for instance, Deza *et al.*^[12] proposed an observer based on a Kalman filter for distillation columns. However, the robustness of the numerical resolution of the differential Riccati equation is not guaranteed. Other authors have used extended Luenberger observers,^[18,19] but the proposed designs use a coordinate transformation to update the observer gain. This implies that the observer design becomes impractical for systems with a large number of differential equations (complexity of calculus of the Jacobian matrix). In Ref.^[20] the authors proposed an observer based on the differential geometry theory which is applicable to either observable or detectable systems and is

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characterized by a systematic construction-tuning procedure, the negative aspect related to the development of a nonlinear geometric observer for distillation columns stems from the coordinate transformation on which the estimator algorithm is based. The geometric approach requires a quasi-linearization of the nonlinear system, which is obtained by applying a Lie derivative transformation to the measured outputs, with a derivative order depending on the dimension of the state vector and the number of available measured outputs.

In this paper, a simple constant-gain observer is synthesized in a distillation process using a recent approach for the class of nonlinear systems studied in Ref.^[21]. This approach involves a single tuning parameter despite the number of differential equations considered in the model. Authors in Ref. ^[21] show that the proposed observer is stable and simulation results were presented considering an ideal binary mixture composed of methanol–ethanol.

The main interest of this work is the on-line test of this observer in a pilot plant, and to verify if this observer is useful to estimate the plate compositions for a non-ideal mixture composed of ethanol–water, using only two on-line measurements: the condenser and the boiler temperatures.

THE BINARY DISTILLATION COLUMN MODEL

The binary distillation column model is derived from the binary distillation column scheme shown in Fig. 1. There are three principal stages considered in a distillation column (condenser, trays and boiler); for every stage, the balances of energy and material should be formulated as well as the vapor–liquid equilibrium relations of the mixture.

General aspects

The scheme of a typical distillation column is shown in Fig. 1. The binary feeding mixture (molar flow rate, F) is introduced toward the middle of the column (the feeding tray). The distilled product (molar flow rate, D), which mainly contains the light component in liquid phase (a total condenser is assumed), is removed from the top of the column. The bottom product (molar flow rate, B), which contains the heavy component in higher concentration, is removed from the bottom of the column. Part of the overhead product (reflux) is returned into the column to improve purity by manipulating the reflux rate using a three-way valve. Column stages are labeled using an ascent numeration from the condenser to the boiler: $i = 1, \dots, N$. Sections of the column are:

- Condenser, tray $i = 1$.

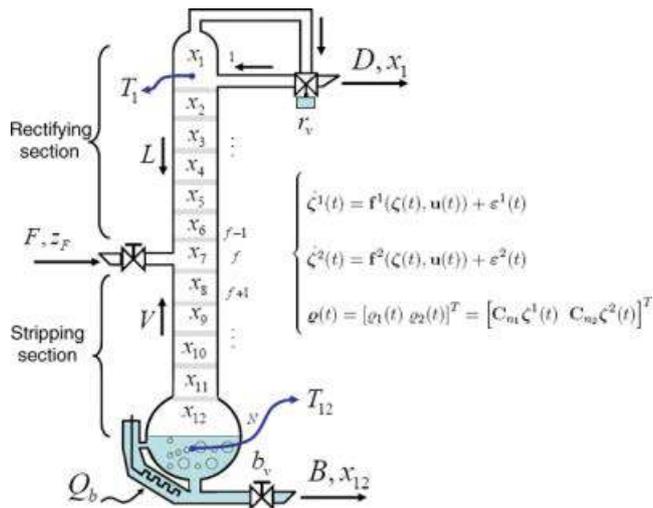


Figure 1. Mathematical model of a distillation column. This figure is available in colour online at www.apjChemEng.com.

- Rectifying section, trays $i = 2, \dots, f - 1$.
- Feeding tray, tray $i = f$.
- Stripping section, trays $i = f + 1, \dots, N - 1$.
- Boiler, tray $i = N$.

Physics behavior

Due to its physical structure, a distillation column can be modeled like a set of interconnected stages using a mass balance and an equilibrium relation at every stage.

The algebraic and differential equations of the model are formulated to calculate the composition of the light component in the liquid and vapor phases (designated by x and y , respectively).

Assumptions

The following assumptions, taken from Ref.^[22,23] are considered in the model formulation:

- (A1) Constant pressure.
- (A2) Ideal liquid–vapor equilibrium.
- (A3) Liquid properties behave as a non-ideal mixture.
- (A4) Negligible molar vapor holdup compared to the molar liquid holdup.
- (A5) Boiler as a theoretical tray.
- (A6) Total condenser.
- (A7) Constant liquid volumetric hold up.

Vapor–liquid equilibrium

If a vapor and a liquid are in intimate contact for a long time period, equilibrium is attained between the two phases. This concept of vapor–liquid equilibrium (VLE) is elemental to model distillation columns. If the vapor–liquid equilibrium exists, then the component vapor composition y and its liquid composition x

can be computed by correlating equations such as $(y^{eq}, x^{eq}) = K(T, P_T)$, where T is the temperature, P_T is the total pressure, y^{eq} and x^{eq} are the vapor and liquid composition of the component at the equilibrium phase, respectively. The equilibrium constant K depends on the thermodynamical properties of the mixture.

The non-ideality of a binary mixture is due to different causes, the most common is the non-ideality of the liquid phase. In consequence, specially designed models are used to represent these non-idealities. For low pressure systems, the equation that represents the vapor composition of the desired component is:

$$yP_T = P^{sat}x\gamma \quad (1)$$

where P^{sat} is the vapor partial pressure and γ is the activity coefficient of the component in every stage. This is a correction factor highly dependent on the concentration. In this work the vapor composition is calculated as a function of the light component (ethanol). One method to determine this coefficient uses the Van Laar equation:

$$\begin{cases} \ln\gamma_{EOH} = A_{12}\left(\frac{A_{21}(1-x)}{A_{12}x+A_{21}(1-x)}\right)^2 \\ \ln\gamma_{H2O} = A_{21}\left(\frac{A_{12}x}{A_{12}x+A_{21}(1-x)}\right)^2 \end{cases} \quad (2)$$

where A_{12} and A_{21} are two interaction parameters established for a binary mixture and x is the liquid composition. Their values for the ethanol–water mixture can be found in Ref.^[24].

Mass transfer effects

In order to deal with the mass transfer effects, the Murphree's efficiencies are introduced. The Murphree stage efficiency E_i is the ratio between the current change in vapor composition between two stages and the change that will occur if the vapor is in equilibrium with the liquid leaving the stage.

In mathematical form the Murphree's efficiencies for the stripping section are given by

$$E_i = \frac{y_i - y_{i+1}}{y_i^{eq} - y_{i+1}}, \quad i = f, f+1, \dots, N-1 \quad (3)$$

and $E_N = 1$ considering assumption (A5).

In the rectifying section, the Murphree efficiency e_i is defined with respect to the liquid phase:

$$e_i = \frac{x_i - x_{i-1}}{x_i^{eq} - x_{i-1}}, \quad i = 2, 3, \dots, f-1 \quad (4)$$

Molar flow rates

In the rectifying section the vapor molar flow V_R and the liquid molar flow L_R are:

$$\begin{cases} V_R = V_S + (1 - q_F)F, & i = 1, \dots, f \\ L_R = (1 - r_v)V_R, & i = 1, \dots, f-1 \end{cases} \quad (5)$$

where

$$q_F = 1 + \frac{C_p(T_b - T_F)}{\lambda} \quad (6)$$

q_F describes the feeding condition according to Table 1, r_v is a binary variable representing the reflux valve position (a three way ON-OFF valve), i.e. $r_v = 0$ means that $L_R = V_R$ and $r_v = 1$ means that $L_R = 0$ (see Fig. 1).

In Eq. (6) C_p is the specific heat, T_b is the boiling temperature, T_F is the feeding temperature and λ is the vaporization enthalpy.

F is the molar flow of the feeding stream

$$F = F_V[\rho_{EOH}w_{EOH} + \rho_{H2O}(1 - w_{EOH})] \times \left(\frac{x_f}{MW_{EOH}} + \frac{1 - x_f}{MW_{H2O}} \right) \quad (7)$$

where F_V is the volumetric flow of the feeding stream, ρ_{EOH} , ρ_{H2O} are densities and MW_{EOH} , MW_{H2O} are molecular weights (subscripts *EOH* and *H2O* denotes ethanol and water respectively). w_{EOH} is the weight fraction of the light component given by

$$w_{EOH} = \frac{x_f \rho_{EOH}}{x_f \rho_{EOH} + (1 - x_f) \rho_{H2O}} \quad (8)$$

The distilled product flow rate, D is given by $D = V_R r_v$, where r_v is a binary variable representing the reflux valve opening, i.e. $r_v = 0$ means that $D = 0$ and $r_v = 1$ means that $D = V_R$.

In the stripping section, the vapor molar flow V_S and the liquid molar flow L_S are, respectively

$$\begin{aligned} V_S &= \frac{Q_b}{\lambda_{EOH}x_N + \lambda_{H2O}(1 - x_N)}, & i = f+1, \dots, N \\ L_S &= L_R + q_F F, & i = f, \dots, N \end{aligned} \quad (9)$$

where Q_b is the heating power on the boiler. Finally, the molar flow rate of the bottom product is:

$$B = (L_S - V_S)b_v$$

Table 1. Feeding condition.

Value	Vaporization degree
$q_F < 0$	Superheated vapor
$q_F = 0$	Saturated vapor
$0 < q_F < 1$	Liquid and vapor
$q_F > 1$	Subcooled liquid
$q_F = 1$	Saturated liquid

where b_v is a binary variable representing the bottom valve opening, *i.e.*

$$b_v = \begin{cases} 0, & (\text{if batch distillation is performed}) \\ 1, & (\text{if the bottom product is withdrawn from the boiler}) \end{cases}$$

The dynamic model

Tray and distilled product compositions are estimated by using the dynamic model based on material, component and energy balances. Taking into account the assumptions (A1) to (A7), a set of differential equations can be derived for the material balance of the light component at each tray:^[25]

$$\begin{cases} \frac{dM_1}{dt} = V_2 - L_1 - D \\ \frac{dM_i}{dt} = V_{i+1} - L_i - V_i + L_{i-1} + \delta(i)F, & i = 2, 3, \dots, N-1 \\ \frac{dM_N}{dt} = L_{N-1} - V_N - B \end{cases} \quad (10)$$

The component balances for each stage are given by

$$\begin{cases} \frac{d(M_1 x_1)}{dt} = V_2 y_2 - L_1 x_1 - D x_1 \\ \frac{d(M_i x_i)}{dt} = V_{i+1} y_{i+1} - L_i x_i - V_i y_i + L_{i-1} x_{i-1} + \delta(i)F z_f \\ \frac{d(M_N x_N)}{dt} = L_{N-1} x_{N-1} - V_N y_N - B x_N \end{cases} \quad (11)$$

where

$$\delta(i) = \begin{cases} 1 & \text{if } i = f \\ 0 & \text{if } i \neq f \end{cases}$$

z_f is the molar composition of the feeding stream given by

$$z_f = \left(\frac{v_{EOH} \rho_{EOH} / MW_{EOH}}{v_{EOH} \rho_{EOH} / MW_{EOH} + v_{H_2O} \rho_{H_2O} / MW_{H_2O}} \right) \quad (12)$$

where v_{EOH} , v_{H_2O} are the initial volume of each component (ethanol or water) on the feeding container (depicted as D1 in Fig.3).

The molar hold-up for every stage M_i can be approximated as^[26]

$$M_i = v_i \frac{1}{\frac{x_i MW_{EOH}}{\rho_{EOH}} + \frac{(1-x_i) MW_{H_2O}}{\rho_{H_2O}}}; \quad i = 1, \dots, N \quad (13)$$

where v_i are the liquid hold-up volume in the trays.

The enthalpies of the process are considered constant, therefore the energy balance is not taken into account to develop this model.

OBSERVER DESIGN FOR A CLASS OF NONLINEAR TRIANGULAR SYSTEMS

The following notation will be used in the rest of the paper: bold letters denote vectors or matrices; the superscript T denotes matrix transpose.

Consider the following nonlinear system written in a compact form:

$$\begin{cases} \dot{\zeta}^1(t) = \mathbf{f}^1(\zeta(t), \mathbf{u}(t)) + \mathbf{e}^1(t) \\ \dot{\zeta}^2(t) = \mathbf{f}^2(\zeta(t), \mathbf{u}(t)) + \mathbf{e}^2(t) \\ \mathbf{q}(t) = [\varrho_1(t) \ \varrho_2(t)]^T = [\mathbf{C}_{n_1} \zeta^1(t) \ \mathbf{C}_{n_2} \zeta^2(t)]^T \end{cases} \quad (14)$$

where $\zeta^1(t) \in \mathcal{R}^{n_1}$, $\zeta^2(t) \in \mathcal{R}^{n_2}$, are the state vectors of the system, such that $n_1 + n_2 = n$ is the order of the system (n_j , $j = 1, 2$, is the size of every state vector $\zeta^j(t)$). Superscripts 1 and 2 are used to denote subvectors, *i.e.* $\zeta(t) = [\zeta^1(t) \ \zeta^2(t)]^T \in \mathcal{R}^n$, whereas subscripts are used to denote the elements of a vector, *i.e.* $\zeta^j(t) = [\zeta_1^j(t), \zeta_2^j(t), \dots, \zeta_{n_j}^j(t)]^T$.

$\mathbf{u}(t) \in \mathcal{R}^m$ is the input vector; $\mathbf{e}^j(t) \in \mathcal{R}^{n_j}$, $j = 1, 2$ are two unknown and bounded disturbance vectors; $\mathbf{q}(t) = [\varrho_1(t) \ \varrho_2(t)]^T \in \mathcal{R}^2$ is the measured output vector. $\mathbf{C}_{n_j} = [1 \ 0 \ \dots \ 0] \in \mathcal{R}^{n_j}$, $j = 1, 2$, then the expression $\mathbf{C}_{n_j} \zeta^j(t)$, $j = 1, 2$ means that only the first element of vector $\zeta^j(t)$, $j = 1, 2$ is measurable, *i.e.* $\varrho_j(t) = \zeta_1^j(t)$, $j = 1, 2$. Finally, the vectors $\mathbf{f}^j(t)$, $j = 1, 2$ have the following triangular structure (the time dependency is omitted for the sake of simplicity):

$$\mathbf{f}^1(\zeta, \mathbf{u}) = \begin{bmatrix} f_1^1(\zeta_1^1, \zeta_2^1, \mathbf{u}) \\ f_2^1(\zeta_1^1, \zeta_2^1, \zeta_3^1, \mathbf{u}) \\ \vdots \\ f_{n_1-1}^1(\zeta^1, \mathbf{u}) \\ f_{n_1}^1(\zeta, \mathbf{u}) \end{bmatrix}$$

and

$$\mathbf{f}^2(\zeta, \mathbf{u}) = \begin{bmatrix} f_1^2(\zeta_1^2, \zeta_2^2, \mathbf{u}) \\ f_2^2(\zeta_1^2, \zeta_2^2, \zeta_3^2, \mathbf{u}) \\ \vdots \\ f_{n_2-2}^2(\zeta_1^2, \dots, \zeta_{n_2-1}^2, \mathbf{u}) \\ f_{n_2-1}^2(\zeta^2, \mathbf{u}) \\ f_{n_2}^2(\zeta, \mathbf{u}) \end{bmatrix}$$

The following assumptions are considered in order to design the observer:

- (A8) $\mathbf{f}^j(t)$ is globally Lipschitz with respect to $\boldsymbol{\zeta}(t)$.
- (A9) The state variables $\boldsymbol{\zeta}(t)$ are bounded

Consider the following notation:

$$\mathbf{A}_{n_j}(t) = \begin{bmatrix} 0 & a_1(t) & 0 & 0 \\ \vdots & & a_2(t) & 0 \\ 0 & & \ddots & a_{n_j-1}(t) \\ 0 & \dots & 0 & 0 \end{bmatrix} \quad (15)$$

where $a_k(t)$, $k = 1, \dots, n_j - 1$ are bounded and unknown functions satisfying the following assumption:

- (A10) There are two finite real numbers α , β with $\alpha > 0$, $\beta > 0$ such that $\alpha \leq a_k(t) \leq \beta$.

Lemma As in Ref.^[21] assume that (A10) hold, then for every $\sigma_j > 0$, $j = 1, 2$ there exists a $n_j \times n_j$ Symmetric Positive Definite (S.P.D.) constant matrix \mathbf{S}_{n_j} and $\exists \eta_j > 0$ such that

$$\mathbf{A}_{n_j}^T(t)\mathbf{S}_{n_j} + \mathbf{S}_{n_j}\mathbf{A}_{n_j}(t) - \sigma_j \mathbf{C}_{n_j}^T \mathbf{C}_{n_j} \leq -\eta_j \mathbf{I}_{n_j}; \quad \forall t \geq 0; j = 1, 2 \quad (16)$$

where $\mathbf{A}_{n_j}(t)$ is given by Eqn (15), \mathbf{I}_{n_j} is the $n_j \times n_j$ identity matrix, and

$$\mathbf{S}_{n_j} = \begin{bmatrix} s_{11} & s_{12} & 0 & & 0 \\ s_{12} & s_{22} & \ddots & & \vdots \\ 0 & \ddots & & \ddots & 0 \\ \vdots & & & \ddots & s_{(n_j-1)n_j} \\ 0 & \dots & 0 & s_{(n_j-1)n_j} & s_{n_j n_j} \end{bmatrix}$$

Assume that the system given in Eqn (14) satisfies hypothesis (A8) to (A10). The following theorem is given:

Theorem Denote by ε the least upper bound of $\|\mathbf{e}^j(t)\|$, $j = 1, 2$, i.e. $\varepsilon = \sup_{t \geq 0} \|\mathbf{e}^j(t)\|$ (sup denotes the supremum). Let δ_1 , δ_2 be two strictly positive constants such that

$$\frac{2n_1 - 1}{2n_2 + 1} \delta_1 < \delta_2 < \frac{2n_1 + 1}{2n_2 - 1} \delta_1; \quad (17)$$

and $\Delta_{\theta^{\delta_j}} = \text{diag}(\theta^{\delta_j}, \theta^{2\delta_j}, \dots, \theta^{n_j \delta_j})$, $j = 1, 2$. Then, there exist two S.P.D. matrices \mathbf{S}_{n_j} , $j = 1, 2$ given by **Lemma** such that the system

$$\begin{cases} \dot{\hat{\boldsymbol{\zeta}}}^1 = \mathbf{f}^1(\hat{\boldsymbol{\zeta}}^1, \mathbf{u}) - r_1 \Delta_{\theta^{\delta_1}} \mathbf{S}_{n_1}^{-1} \mathbf{C}_{n_1}^T (\mathbf{C}_{n_1} \hat{\boldsymbol{\zeta}}^1 - \varrho_1) \\ \dot{\hat{\boldsymbol{\zeta}}}^2 = \mathbf{f}^2(\hat{\boldsymbol{\zeta}}^2, \mathbf{u}) - r_2 \Delta_{\theta^{\delta_2}} \mathbf{S}_{n_2}^{-1} \mathbf{C}_{n_2}^T (\mathbf{C}_{n_2} \hat{\boldsymbol{\zeta}}^2 - \varrho_2) \end{cases}$$

is an observer for the system given in Eqn (14) if $\exists r_1 > 0$, $\exists r_2 > 0$, $\exists \theta > 0$, $\exists v_1 > 0$, $\exists v_2 > 0$, $\exists \mu > 0$, such that $\forall \hat{\boldsymbol{\zeta}}(0)$, $\boldsymbol{\zeta}(0)$:

$$\|\hat{\boldsymbol{\zeta}}(t) - \boldsymbol{\zeta}(t)\| \leq v_1 e^{-\mu t} \|\hat{\boldsymbol{\zeta}}(0) - \boldsymbol{\zeta}(0)\| + v_2 \varepsilon \quad (19)$$

Remark If $\varepsilon \neq 0$, the estimation error $\mathbf{e}_r = \hat{\boldsymbol{\zeta}}(t) - \boldsymbol{\zeta}(t)$ lies in a ball $B(0, v_2 \varepsilon)$, however, if $\varepsilon = 0$, the estimation error \mathbf{e}_r converges toward $\mathbf{0} \in \mathcal{R}^n$ in a finite time. A complete proof of this result is given in Ref. ^[21].

APPLICATION OF THE OBSERVER TO A DISTILLATION COLUMN

The model in nonlinear state-space form

The dynamical mathematical model of the distillation column is a set of N coupled nonlinear differential equations given in Eqn (11) (considering Eqn (13), the material balance given in Eqn (10) become algebraic equations). A straightforward simplification is obtained if the Lewis hypothesis is considered, which implies that vapor and liquid flow rates are constant along the stripping section and the rectification section. In this work all the mixture was placed initially in the boiler and the feed flow rate was not considered (semi-batch distillation, $F = 0$, $z_f = 0$). Then $L = L_1 = L_2 = \dots = L_{N-1}$, $V = V_2 = V_3 = \dots = V_N$.

The states of the model are the liquid compositions x_i ($i = 1, \dots, N$). They can be classified in two vectors:

$$\mathbf{x}^1(t) = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{j-1} \end{bmatrix} \quad \mathbf{x}^2(t) = \begin{bmatrix} x_N \\ x_{N-1} \\ \vdots \\ x_j \end{bmatrix}$$

where clearly $n_1 + n_2 = N$. Physically, the elements of the vectors $\mathbf{x}^1(t)$ and $\mathbf{x}^2(t)$ represent the liquid concentrations in the rectifying and the stripping section respectively.

The two control variables are $\mathbf{u}(t) = [u_1(t) \ u_2(t)]^T = [V \ L]^T$. These input variables can be manipulated by varying the heating power applied on the boiler $Q_b(t)$ and the opening period of the reflux valve $r_v(t)$ respectively.

If the top and the bottom product compositions x_1 and x_N can be measured, then the measured output vector is

$$\boldsymbol{\varrho}(t) = [\varrho_1(t) \ \varrho_2(t)]^T = [x_1(t) \ x_N(t)]^T$$

This notation leads to the following compact representation of the dynamical mathematical model of the distillation column:

$$\begin{aligned}\dot{\mathbf{x}}^1(t) &= \mathbf{f}^1(\mathbf{x}(t), \mathbf{u}(t)) \\ \dot{\mathbf{x}}^2(t) &= \mathbf{f}^2(\mathbf{x}(t), \mathbf{u}(t)) \\ \boldsymbol{\varrho}(t) &= [\mathbf{C}_{n_1} \mathbf{x}^1(t) \ \mathbf{C}_{n_2} \mathbf{x}^2(t)]^T\end{aligned}\quad (20)$$

where $\mathbf{x}(t) = [\mathbf{x}^1(t) \ \mathbf{x}^2(t)]^T \in \mathcal{R}^n$, $n = N$ and

$$\mathbf{f}^1(\mathbf{x}, \mathbf{u}) = \begin{bmatrix} f_1^1(x_1^1, x_2^1, \mathbf{u}) \\ f_2^1(x_1^1, x_2^1, x_3^1, \mathbf{u}) \\ \vdots \\ f_{n_1-1}^1(\mathbf{x}^1, \mathbf{u}) \\ f_{n_1}^1(\mathbf{x}, \mathbf{u}) \end{bmatrix}$$

$$\mathbf{f}^2(\mathbf{x}, \mathbf{u}) = \begin{bmatrix} f_1^2(x_1^2, x_2^2, \mathbf{u}) \\ f_2^2(x_1^2, x_2^2, x_3^2, \mathbf{u}) \\ \vdots \\ f_{n_2-2}^2(x_1^2, \dots, x_{n_2-1}^2, \mathbf{u}) \\ f_{n_2-1}^2(\mathbf{x}^2, \mathbf{u}) \\ f_{n_2}^2(\mathbf{x}, \mathbf{u}) \end{bmatrix}$$

$$\mathbf{C}_{n_j} = [1 \ 0 \ 0 \ \dots \ 0] \quad (j = 1, 2)$$

Clearly, the system in Eqn (20) have the same form than Eqn (14) where $\boldsymbol{\zeta}(t) = \mathbf{x}(t)$ and $\boldsymbol{\varepsilon}^j(t) = \mathbf{0}$, $j = 1, 2$ (usually F and z_f are considered disturbances, see for instance Ref.^[27]), then the following system is an observer for the distillation column (assumptions **(A8)**–**(A10)** are fulfilled, see Ref.^[21]):

$$\begin{cases} \dot{\hat{\mathbf{x}}}^1 = \mathbf{f}^1(\hat{\mathbf{x}}, \mathbf{u}) - \mathbf{Q}_{1\theta}(\mathbf{C}_{n_1} \hat{\mathbf{x}}^1 - \boldsymbol{\varrho}_1) \\ \dot{\hat{\mathbf{x}}}^2 = \mathbf{f}^2(\hat{\mathbf{x}}, \mathbf{u}) - \mathbf{Q}_{2\theta}(\mathbf{C}_{n_2} \hat{\mathbf{x}}^2 - \boldsymbol{\varrho}_2) \end{cases}\quad (21)$$

where $\mathbf{Q}_{j\theta} = r_j \Delta_{\theta^{\frac{1}{n_j}}} \mathbf{S}_{n_j}^{-1} \mathbf{C}_{n_j}^T$, for $j = 1, 2$.

Observer experimental validation

Distillation pilot plant description

The distillation pilot plant, located at the Process Control Laboratory of the National Center of Technological Research and Development (CENIDET) in Cuernavaca, Morelos, Mexico, where the experiments were carried out is shown in Fig. 2. It has 12 trays, where temperature measurements are available through 8 Resistance Temperature Detectors (RTDs) Pt-100 located at trays 1, 2, 4, 6, 7, 9, 11 and 12. Using these measurements



Figure 2. The distillation pilot plant interacting with the monitoring station (PC). This figure is available in colour online at www.apjChemEng.com.

and considering the equilibrium relation (see section on Vapor–Liquid Equilibrium), the respective liquid compositions can be obtained.

The instruments of the distillation column (an instrumentation diagram is shown in Fig. 3) are connected to two Digitric 500 controllers.^[28] These instruments of the column allow controlling:

- the flow of the cooling liquid through the pneumatic valve (FV1) and the flow controller (FC1).
- the residual pressure of the plant, which provides the possibility to operate the column at values lower than atmospheric pressure; through the pneumatic valve (PV1), the vacuum pump (G2) and the pressure controller (PC1).
- the feeding mixture temperature through a pre-heating electric thermo-coil (J1).
- the feeding mixture doses through the feeding pump (G1).

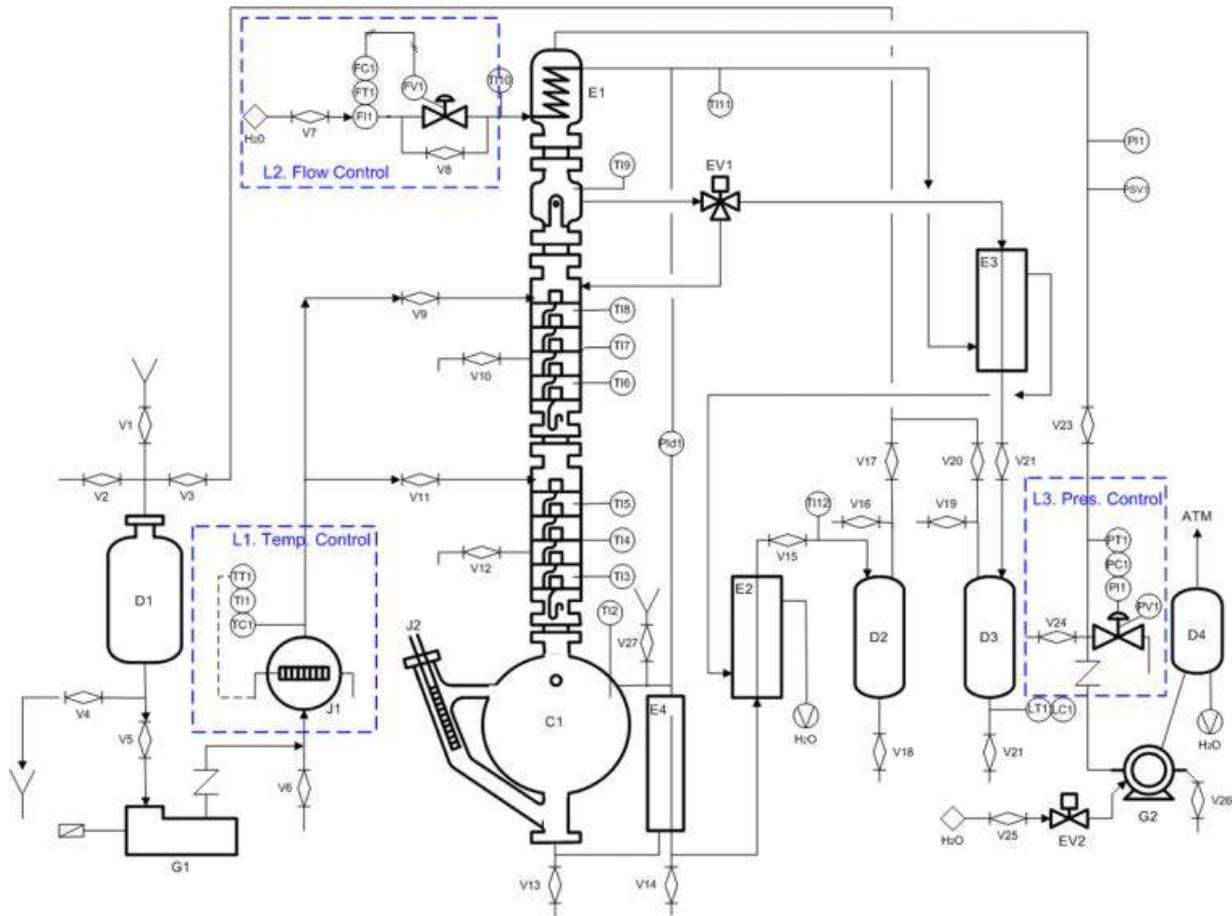


Figure 3. Distillation column instrumentation. This figure is available in colour online at www.apjChemEng.com.

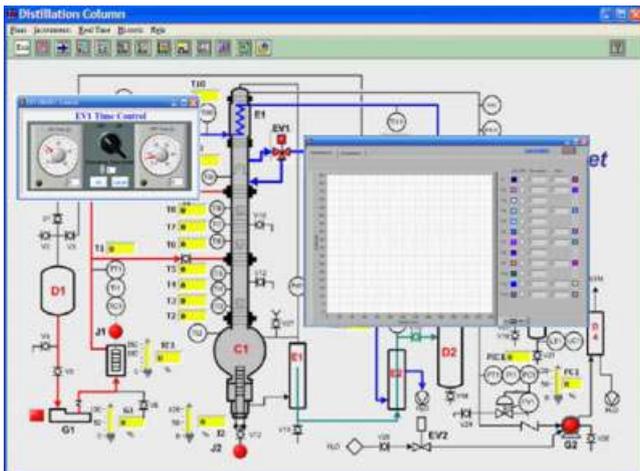


Figure 4. Monitoring station (no data). This figure is available in colour online at www.apjChemEng.com.

The monitoring station allows controlling the column, as well as monitoring the measured temperatures on-line. The main window (user interface) of the station is shown in Fig. 4.

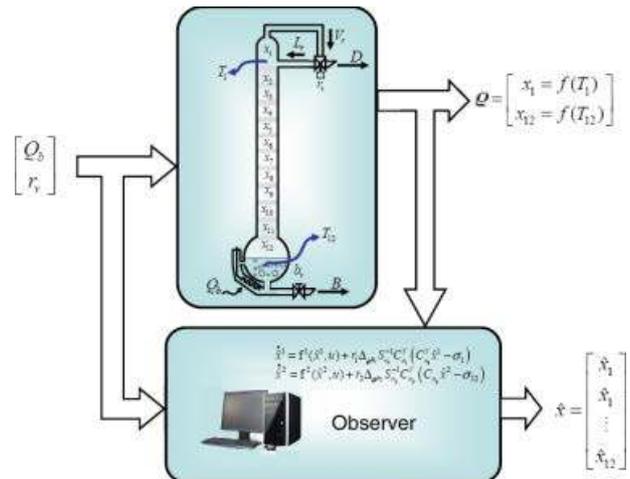


Figure 5. Observer on-line implementation. This figure is available in colour online at www.apjChemEng.com.

High-gain observer tuning

The observer shown in Eqn (21) was implemented in the process control interface system described in Ref.^[29]

Figure 5 shows the block diagram of the observer-interface configuration.

This observer estimates the liquid composition of the light component (*EOH*) for every stage by having the temperature measurements on stage 1 (condenser) and stage 12 (boiler).

The high-gain observer is obtained by fixing $r_1 = r_2 = 25$; $\theta = 0.09$ and satisfying (21) with $\delta_1 = 1.2$, $\delta_2 < \frac{2m+1}{2n_2-1}\delta_1 = 1.38$ (where $n_1 = f - 1 = 6$, $n_2 = n - f + 2 = 6$). Finally the Lemma gives:

$$\mathbf{S}_{n_j} = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1.5 & 0 & 0 & 0 \\ 0 & -1.5 & 4 & -2 & 0 & 0 \\ 0 & 0 & -2 & 8 & -3 & 0 \\ 0 & 0 & 0 & -3 & 10.5 & -4 \\ 0 & 0 & 0 & 0 & -4 & 15.5 \end{bmatrix}$$

The observer convergence speed may be chosen arbitrarily; if θ is large, then the convergence time becomes shorter. Although if θ is large enough, then the observer becomes more measurement-noise sensitive (measurement-noise means the deviation of the measured (observed) value from the true value). The tuning of nonlinear observers is still theoretically difficult to achieve, then only simulations and/or on-site experiments allow obtaining an adequate compromise between the fast convergence of the observer and its measurement-noise sensitivity.

Experimental results

Different experiments were developed in order to validate the on-line performance of the observer, considering the convergence time and the estimated states accuracy as the main validation parameters. Obtained results were similar during these different experiments therefore only one is reported in this paper.

The mixture used in these experiments was ethanol (*EOH*) and water (H_2O) which is considered a non-ideal mixture. The physical specifications of the components of the binary mixture are presented in Table 2.

The experimental validation of the observer given in Eqn (21) is done considering: *EOH* volume of 2000 ml, H_2O volume of 2000 ml and process total pressure of 105.86 kPa.

Table 2. Specifications of the components of the mixture ethanol–water.

Parameter	Ethanol	Water	Units
Density (ρ)	0.789	1	g/cm^3
Molecular weight (MW)	46.069	18.015	g
Boiling temperature (T_b)	78.400	100	$^\circ C$
Vaporization enthalpy (H_{vap})	38.560	40.650	kJ/mol
Specific heat (C_p)	0.112	0.076	$kJ/mol\ ^\circ C$

Table 3. Process inputs.

Input	Signal	Start time
Q_b	Step 0 – 1000 W	0 min
Reflux	Total	0 min
Q_b	Step 1000 – 1250 W	18 min
Reflux	Pulse($t_{on} = t_{off} = 6$ s)	38 min
Reflux	Total	69 min

The observer initial conditions for the light component composition were:

$$\hat{\mathbf{x}}^1(0) = [0.862 \ 0.860 \ 0.744 \ 0.743 \ 0.740 \ 0.641]$$

$$\hat{\mathbf{x}}^2(0) = [0.163 \ 0.371 \ 0.560 \ 0.574 \ 0.641]$$

The temperature measurements available at trays 1, 2, 4, 6, 7, 9, 11 and 12 were used to estimate the respective liquid compositions as measured data (see section on Vapor–Liquid Equilibrium). The VLE curve was adjusted using off-line measurements of the composition, which were performed using an adequate alcoholometer.

Since the results obtained for all the trays are quite similar, only those related to five of them are presented: the condenser (tray 1), tray 4 in the rectifying section, the feeding tray, tray 9 in the stripping section and the boiler (tray 12).

The selected sampling time was 3 s and the time the experiment lasts was 88 min once it had reached the steady-state. In the 38th minute, a change in the input Q_b is applied. In the 68th minute, the system goes from total reflux to partial reflux. These inputs changes are shown in Table 3.

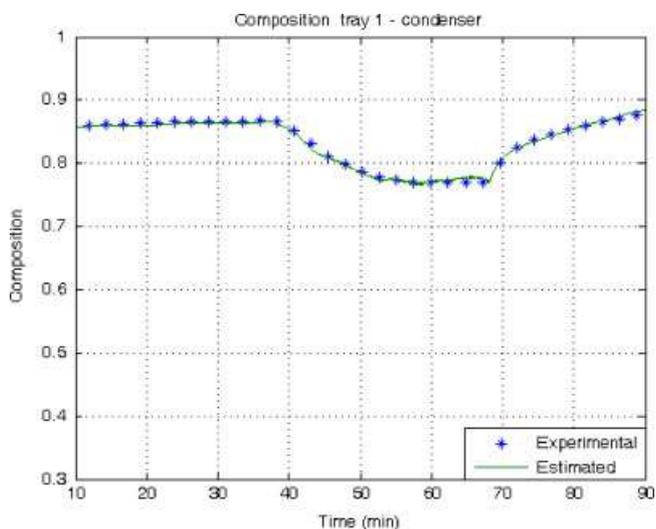


Figure 6. Measured and estimated composition of *EOH* at the condenser. This figure is available in colour online at www.apjChemEng.com.

Figures 6 to 10 show a comparison between the estimated composition and the composition obtained by using the measured temperatures (experimental data). In these figures good tracking and quick convergence of the observer to the experimental data can be seen. Therefore, it can be assumed that this observer is adequate to estimate the compositions of the light component in the binary mixture of ethanol–water accurately.

An important aspect that makes this case study interesting is that the equilibrium temperature does not change significantly when the ethanol mole fraction in the liquid phase changes from 0.33 to 0.87; in particular,

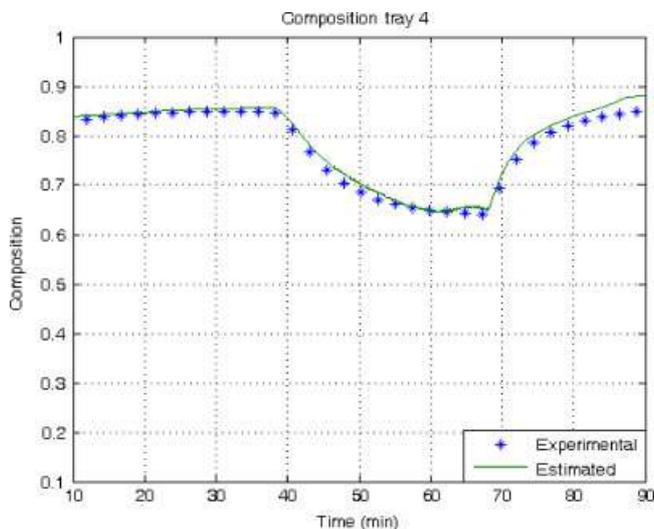


Figure 7. Measured and estimated composition of EOH at tray 4 (rectifying section). This figure is available in colour online at www.apjChemEng.com.

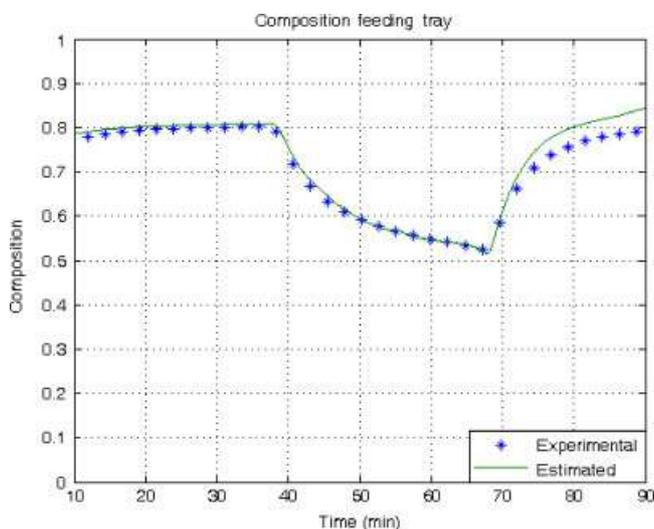


Figure 8. Measured and estimated composition of EOH at the feeding tray. This figure is available in colour online at www.apjChemEng.com.

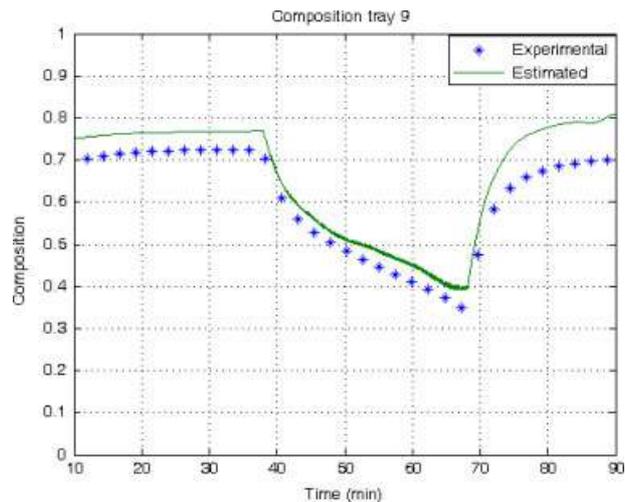


Figure 9. Measured and estimated composition of EOH at tray 9 (stripping section). This figure is available in colour online at www.apjChemEng.com.

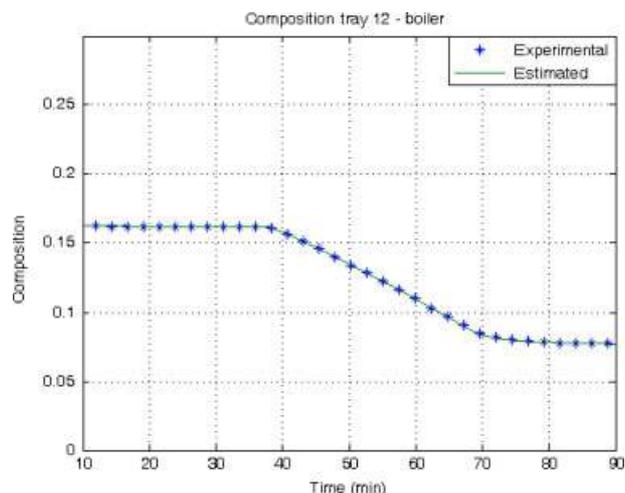


Figure 10. Measured and estimated composition of EOH at the boiler. This figure is available in colour online at www.apjChemEng.com.

the temperature varies by 3°C approximately within this mole fraction interval, with a 0.3°C variation in the interval from 0.548 to 0.87. This implies that a small error (or noise) in the measured temperature output can lead to a large error in the top composition estimation. On the other hand, at high ethanol dilution on the bottom, the temperature is very sensitive to composition changes and measurement noise has a much lower impact on the estimation.

CONCLUSIONS

In this paper a nonlinear observer for a special class of multi-output nonlinear system has been presented.

The nonlinear observer was synthesized by using a very simple model of a binary distillation column (ethanol–water) and used to estimate on-line (by using a process control interface developed for this end) the ethanol composition at each tray in the column, based only on temperature measurements in the condenser and the boiler.

Although this observer was proposed previously in Ref. [21] there are not previous works covering the on-line implementation in a real pilot plant. By doing that, an interesting conclusion arises: this nonlinear observer can be used not only to estimate the plate compositions of ideal mixtures, but composition estimation can also be performed for non-ideal mixtures by using simple models rather than very complicated models involving a large number of phenomenons. That means, the correction term of the observer $\mathbf{Q}_{j\theta}(\mathbf{C}_{nj}\hat{\mathbf{x}}^1 - \mathbf{q}_j)$, ($j = 1, 2$) in Eqn (18) compensates well the difference between the model and the real process.

The main advantage of this kind of correction term is that the gains $\mathbf{Q}_{j\theta}$, ($j = 1, 2$) are constants and explicitly given. This feature avoid to compute dynamically the gains (such is the case in observers based on Kalman filters, where the solution of the differential Riccati equations can be very time consuming for this kind of nonlinear systems involving several state variables) and then the algorithm becomes faster and easier to be tuned.

NOMENCLATURE

Capital letters

A_{12}	Van Laar constant
A_{21}	Van Laar constant
B	Bottom product flow, mol/min
C_p	Specific heat, $kJ/mol^\circ C$
D	Distilled product, mol/min
E	Murphree's efficiency
F	Molar flow of the feeding stream, mol/min
F_V	Volumetric flow of the feeding stream, mL/min
K	Equilibrium constant
L	Liquid molar flow, mol/min
L_R	Liquid molar flow (rectifying section), mol/min
L_S	Liquid molar flow (stripping section), mol/min
M	Molar hold-up, mol
MW	Molecular weight, g
N	Number of trays
P^{sat}	Partial pressure (saturation), kPa
P_T	Total pressure, kPa
Q_b	Heating power, $Watts$
T	Temperature, $^\circ C$
T_b	Boiling temperature, $^\circ C$
T_F	Feeding temperature, $^\circ C$
V	Vapor molar flow, mol/min
V_R	Vapor molar flow (rectifying section), mol/min

V_S Vapor molar flow (stripping section), mol/min

Lowercase letters

b_v	Bottom valve opening, [0, 1]
i	Tray number
e	Murphree's efficiency
f	Feeding tray
q_F	Quality of the feed
r_v	Reflux valve opening, [0, 1]
v	Volume ml^3
w	Weight fraction
x	Liquid compositions
x^{eq}	Liquid compositions in equilibrium
y	Vapor compositions
y^{eq}	Vapor compositions in equilibrium
z_f	Feed composition

Greek letters

γ	Activity coefficient
λ	Vaporization enthalpy, kJ/mol
ρ	Component density, g/cm^3

Subscripts

EOH	Ethanol
H_2O	Water
N	Number of trays
i	Tray number
f	Feeding tray
R	Rectifying section
S	Stripping section

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