Composition estimation of a six-component distillation column with temperature measurements

Andrea Frau, * **Roberto Baratti,** * **Jesús Alvarez** **

* *Dipartimento di Ingegneria Chimica e Materiali, Università degli Studi di Cagliari, Piazza d'Armi, 09123 Cagliari*
** *Universidad Autónoma Metropolitana-Iztapalapa, Depto. De Ingegneria de Procesos e Hidraúlica, Apdo. 55534, 09340 México D.F. México*

Abstract: The problem of jointly designing the estimation structure and algorithm to infer all or some composition in a six-component distillation column with temperature measurements is addressed. The structure design involves the choices of: (i) modeled and unmodeled compositions, (ii) the number of measurements and their location, and (iii) the innovated-noninnovated state partition. The algorithm is the dynamic data processor that performs the estimation task. The application of the geometric estimation approach (GE), in the light of the column characteristics, yields a tractable procedure to draw the solution of the estimation structure-algorithm design problem, with an estimation scheme that is considerably simpler than previous ones with extended Kalman Filter (EKF). The proposed methodology is applied to a representative six-component case example through simulations, finding that the estimation task can be performed with a three-component reduced model.

Keywords: Distillation column, nonlinear, estimators, geometric estimators, multicomponent.

1. INTRODUCTION

Distillation is an important energy-intensive industrial operation where many substances are separated and purified. The development of estimation schemes with temperature measurements for multicomponent distillation columns is motivated by: (i) the need of developing monitoring systems and (supervisory, advisory, and feedback) controllers with applicability-oriented requirements on reliability, tractability and maintenance cost, and (ii) the availability of reasonable and reliable multicomponent distillation models, including commercial packages.

The extended Kalman Filter (EKF) (Jazwinsky (1970)) has been by far the most widely used estimation technique in chemical process systems engineering in general, and in multicomponent distillation columns in particular, with successful simulations and experimental implementations for continuous and batch column operations, mostly for binary (Baratti et al. (1995); Yang and Lee (1997)) and ternary systems (Baratti et al. (1998)), and up to four-component systems (Venkateswarlu and Kumar (2006)). Even though adequate multicomponent column models are available, the related EKF construction and implementation for multicomponent systems still rises reliability, complexity, and development-maintenance cost concerns among industrial practitioners, because: (i) the dimensionality of the EKF grows rapidly with the number of stages and components ($\frac{n(n+1)}{2}+n$), (ii) the tuning of the covariance gains of the Riccati equation is a rather complex task, and (iii) due to the lack of formal connections between estimator tuning and functioning, the implementation of the EKF requires extensive testing.

Recently, the geometric estimation (GE) approach (Alvarez (2000)), which does not require the on-line integration of Riccati equations, has been redesigned with the following features (Alvarez and Fernandez (2008)): (i) the obstacle of high order Lie derivations has been removed and replaced by Jacobian model-based gain computations, enabling the consideration of staged systems, (ii) the equivalence between the GE and the EKF has been identified, (iii) the estimation model, its (innovation-noninnovation) detectability structure, and the sensor locations are regarded as structural design degrees of freedom, and (iv) a simple tuning scheme is coupled with a robust convergence criterion. The general-purpose GE approach has been successfully tested with experimental binary columns with complete (Tronci et al. (2005); Fernandez and Alvarez (2007)) or reduced models (Alvarez and Fernandez (2008)), and ternary columns (Pulis et al. (2006)), yielding estimation schemes which are considerably simpler than the EKF-based ones. These considerations motivate the present study on the six-component distillation column problem.

In this work, the problem of simultaneously designing the estimation structure and algorithm to infer all or some composition in a six-component distillation column with temperature measurements is addressed. By structure design we mean the choices of: (i) modeled and unmodeled compositions, (ii) the number of measurements and their locations, and (iii) the innovated-noninnovated composi-

tion state partition which, in conjunction with the model-sensor choice, determines the data assimilation versus error propagation mechanism. By algorithm it is meant the dynamic data processor that performs the estimation task, according to the estimation structure and a suitable gain tuning scheme. The application of afore discussed GE approach, in the light of the six-component column characteristics, yields a tractable procedure to solve the structure-algorithm problem, with an estimation scheme that is considerably simpler than previous EKF-based ones. The proposed methodology is applied to a representative six-component case example through simulations, finding that the estimation task can be performed with a three-component reduced model, a single-stage innovation with passive structure, and without the need of online integrating Riccati equations. The study can be seen as an inductive step towards the consideration of columns with more than six components.

2. ESTIMATION PROBLEM

2.1 Six-component distillation column

Consider a continuous multicomponent column with N stages and C components. Under standard assumptions (energy balance neglected on each tray, constant vapor and liquid flows, holdup dynamics neglected, tight reboiler and condenser level control, and stage liquid-vapor equilibrium), the column dynamics are described by the following set of nonlinear differential equations (Skogestad (1997); Baratti et al. (1998)):

Reboiler ($i = 1$, $j = 1, \ldots, C-1$)

$$\dot{c}_1^j = \frac{(R+F)c_2^j - V\epsilon_j(c_1, P_1) - Bc_1^j}{M_1} = f_1^j(c_1, c_2^j) \quad (1a)$$

Stripping section ($2 \le i \le N_F - 1$, $j = 1, \ldots, C-1$)

$$\dot{c}_i^j = \frac{(R+F)(c_{i+1}^j - c_i^j) - V(\epsilon_j(c_i, P_i) - \epsilon_j(c_{i-1}, P_{i-1}))}{M_i} \quad (1b)$$
$$= f_i^j(c_{i-1}, c_i, c_{i+1}^j)$$

Feed tray ($i = N_F$, $j = 1, \ldots, C-1$)

$$\dot{c}_{N_F}^j = \frac{R(c_{N_F+1}^j - c_{N_F}^j) + F(c_F^j - c_{N_F}^j)}{M_{N_F}} - \frac{V(\epsilon_j(c_{N_F}, P_{N_F}) - \epsilon_j(c_{N_F-1}, P_{N_F-1}))}{M_{N_F}} \quad (1c)$$
$$= f_{N_F}^j(c_{N_F-1}, c_{N_F}, c_{N_F+1}^j, c_F)$$

Enriching section ($N_F + 1 \le i \le N - 1$, $j = 1, \ldots, C-1$)

$$\dot{c}_i^j = \frac{R(c_{i+1}^j - c_i^j) - V(\epsilon_j(c_i, P_i) - \epsilon_j(c_{i-1}, P_{i-1}))}{M_i} \quad (1d)$$
$$= f_i^j(c_{i-1}, c_i, c_{i+1}^j)$$

Condenser ($i = N$, $j = 1, \ldots, C-1$)

$$\dot{c}_N^j = \frac{V\epsilon_j(c_{N-1}, P_{N-1}) - Rc_N^j - Dc_N^j}{M_N} = f_N^j(c_{N-1}, c_N^j) \quad (1e)$$

Temperature measurements ($i = 1, \ldots, m$)

$$T_{s_i} = \beta(c_{s_i}, P_{s_i}) \quad (1f)$$

where m is the number of sensors along the column and s_i is the location of the i-th sensor, c_i^j is the composition of the component j at i-th stage, $c_i = [c_i^1 \ \ldots \ c_i^{C-1}]^T$ is the composition vector at i-th stage, T_{s_i} and P_{s_i} are respectively the temperature and the pressure at s_i-th stage, F is the feed flow rate with composition $c_F = [c_F^1 \ \ldots \ c_F^{C-1}]^T$, D, B, R, and V are respectively the distillate, bottom, reflux and vapor flow rate (V is proportional to reboiler duty Q through the heat of vaporization λ), M_i is the holdup at i-th stage, ϵ_j is the liquid-vapor equilibrium function that determines the vapor composition of the component j, and β is the bubble-point implicit function that sets the temperature. The components c_i^C are determined by the (mass conservation) condition $\sum_{j=1}^{C} c_i^j = 1$, where $i = 1, \ldots, N$. Henceforth, column system (1), will be referred to as the *complete six-component column system*, which in compact vector notation is written as follows:

$$\dot{x}_P = f_P(x_P, u_P, d_P) \qquad y_P = h_P(x_P) \quad (2)$$

where $x_P = [{c_1}^T \ldots {c_N}^T]^T$, $c_i = [c_i^{C2} \, c_i^{C3} \, c_i^{IC4} \, c_i^{NC4} \, c_i^{IC5}]^T$, $u_P = [R \, V]^T$, $d_P = [F \, {c_F}^T]^T$, and $y_P = [T_{s_1} \ \ldots \ T_{s_m}]^T$ are respectively the states, the inputs, the disturbances, and the outputs. The disturbances d_P are assumed to be constant and known.

2.2 Estimation problem

The estimation problem consists in jointly designing the estimation structure (i.e. estimator model, sensor location, innovated states and data assimilation mechanism), and the estimation algorithm (i.e., the dynamic data processor), to infer some of or all the effluent compositions of the six-component distillation column (2) on the basis of a reduced model (to be designed) in conjunction with temperature measurements, according to a specific estimation objective. In virtue of the general-purpose GE approach (Alvarez and Fernandez (2008)) and its applications to binary (Fernandez and Alvarez (2007); Alvarez and Fernandez (2008)) and ternary columns (Pulis et al. (2006)), in the present six-component column estimation study, the emphasis will be placed on: (i) the design of a reduced-component model for estimation, (ii) the employment of a robustness-oriented single-stage innovation scheme with passive structure (Pulis (2007)), (iii) the corresponding decision on the innovated components, meaning the components of the measurement stage with information and error injection, and (iv) the estimation of the effluent (distillate and bottom) impurity compositions as estimation objective.

2.3 Case example

As a representative industrial case example, consider the T110 distillation column located at SARAS refinery (Sarroch, Italy) with $N = 37$ stages and $C = 6$ components: a C3-C4 (propane-butane) splitter fed with propane (C3), iso-butane (IC4), and n-butane (NC4), as well as ethane (C2), iso-pentane (IC5), and n-pentane (NC5) as secondary components (with compositions less than 1%).

The column has a kettle reboiler (1-st stage), a total condenser (37-th stage), 35 nutter float valve trays, the feed is introduced at 19-th stage, the tray spacing is 61 cm, the column diameter is 2 m, and the pressure changes linearly along the column, with the top and bottom pressure being 16.3 Kg·cm^{-2} and 16.6 Kg·cm^{-2}, respectively. This case example represents a sufficiently important class of industrial columns, where two or three main components to be split are present, together with other secondary components in a much smaller amount.

The behavior of the "actual" six-component system (2) was numerically simulated with MATLAB, in the understanding that the same task can be performed with commercial packages (say ASPEN). The thermodynamics was simulated with ideal equilibrium (Reid et al. (1998)). The feed flow and compositions, as well as the reflux flow, and reboiler duty are given in Table 1. In all simulations, the initial conditions for the complete column system correspond to the steady-state determined by the data listed in Table 1.

Table 1. Input values for feed flow and compositions, reflux flow and reboiler duty

F (m^3·h^{-1})	82.9	C2 molar fraction	0.0036
R (m^3·h^{-1})	69.7	C3 molar fraction	0.281
Q (BTU)	19819000	IC4 molar fraction	0.236
		NC4 molar fraction	0.4746
		IC5 molar fraction	0.004
		NC5 molar fraction	0.0008

3. STRUCTURAL ANALYSIS

Motivated by the GE detectability measure-based sensor location criterion employed in previous binary (Tronci et al. (2005); Fernandez and Alvarez (2007); Alvarez and Fernandez (2008)) and ternary columns (Pulis et al. (2006)) as well as by their interpretation in terms of thermodynamic diagrams (Pulis et al. (2006)), in this section the sensor location and innovated composition structure is analyzed on the basis of stage-to-stage temperature gradients and their component-wise contributions.

3.1 Model reduction

The stage-to-stage temperature gradient about a certain operation condition is approximated as follows:

$$\Delta T_i = T_{i+1} - T_i \approx \sum_{j=1}^{C} \left.\frac{\partial T_i}{\partial c_i^j}\right|_{c_i} \Delta c_i^j = \sum_{j=1}^{C} \Delta T_{c_i^j} \qquad (3)$$

where $\Delta c_i^j = c_{i+1}^j - c_i^j$, ΔT_i is the temperature gradient at the i-th stage, and $\Delta T_{c_i^j}$ is the contribution of the i-th gradient due to the component j. The idea which underlies the model reduction criterion is to set a data assimilation scheme with a favorable compromise between data assimilation and error propagation: (i) the stages with large temperature gradients are candidates for robustness-oriented single-stage (i.e. passive) innovation, and (ii) the compositions with large contributions to the overall gradient are candidates for being both modeled states and innovated states.

Table 2. Feed compositions for the reduced model

C3 molar fraction	0.2838
IC4 molar fraction	0.2388
NC4 molar fraction	0.4774

On the basis of the steady-state solution of the complete system (2) in conjunction with the total and per-component temperature gradient formula (3), the diagram presented in Figure 1 was obtained, showing that: (i) with respect to stage-to-stage temperature change, the most sensitive zone is the enriching section around the 32-nd stage, (ii) in general, the temperature gradients are due to C3, IC4 and NC4 composition changes, (iii) the IC5, and NC5 components have a rather small contribution to the temperature gradient, and (iv) at the top of the column (around the condenser stage) the C2 has a rather important influence on temperature.

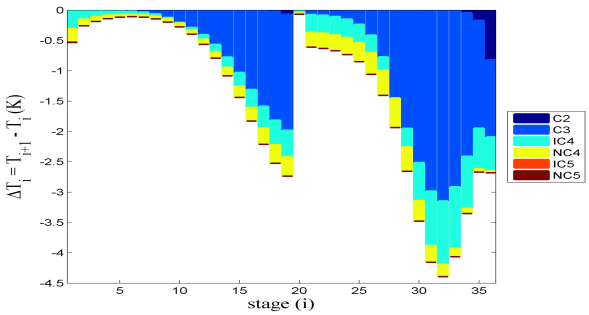

Fig. 1. Complete model-based temperature gradient and its per-component contributions

From the examination of the stage-to-stage temperature gradient and the per-component contributions to such gradient, the following structural conclusions are reached: the reduced model is obtained by retaining the C3, IC4, and NC4 components with appreciable manifestation in the temperature gradient, and discarding the three other ones (C2, IC5, and NC5) with comparatively small manifestation. Thus the reduced model is given by (1) with $C = 3$. In vector notation, the *reduced model* is written as follows:

$$\dot{x} = f(x, u, d) \qquad y = h(x) \qquad (4)$$

where $x = [c_1^{C3} c_1^{IC4} \dots c_N^{C3} c_N^{IC4}]^T$, $u = [RV]^T$, $d = [F c_F^{C3} c_F^{IC4}]^T$, and $y = [T_{s_1} \dots T_{s_m}]^T$ are respectively the states, the inputs, the disturbances, and the outputs. The reduced model (4) was set with the feed compositions presented in Table 2.

The behaviors of the reduced three-component model (4) and complete six-component system (2) are presented in Figure 2, showing that the model reduction error has an appreciable (or negligible) manifestation in the distillate (or bottoms) concentrations, and the same is true for the enriching (or stripping) section. This signifies that: (i) the bottom composition can be adequately estimated, without measurement injection, by means of a reduced model-based open-loop observer, and (ii) the distillate compositions can be estimated with a reduced model-based estimator with one temperature measurement, as

the temperature measurement before the top of the column basically reflects C3 and IC4 changes.

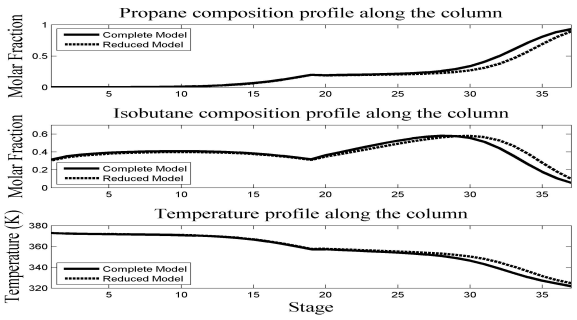

Fig. 2. C3 and IC4 composition and temperature profiles along the column with (six-component) complete and (three-component) reduced models

3.2 Sensor location and innovated states

On the basis of the steady-state solution of the reduced model (4) in conjunction with the total and per-component temperature gradient formula (3), the diagram presented in Figure 3 was obtained, showing that: (i) in the stripping (or enriching) section, the largest temperature gradient, or equivalently, the richest-in-information zone, is located below the feed (or top) tray, and (ii) in the stripping (or enriching) section, the smallest temperature gradient, or equivalently, the poorest-in-information zone, is located above the reboiler (or feed) tray.

From the preceding comments and the findings of Subsection 3.1, the next conclusions on sensor location follow: (i) one temperature measurement should be placed in the stripping section, located at the richest-in-information region (between 29-th and 33-rd stages) with the largest temperature gradient, and (ii) no temperature measurement is needed in the stripping section, as the bottom compositions can be adequately estimated using just the reduced model (without measurements). According to Figure 3, the C3 component has the largest contribution to the temperature gradient in the richest-in-information zone, meaning that the C3 component is an innovated state candidate for a robustness-oriented GE with passive structure (Pulis et al. (2006)).

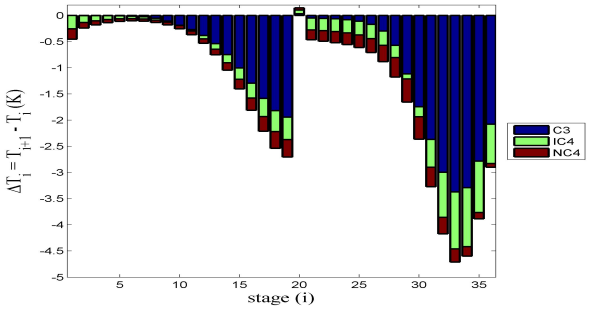

Fig. 3. Reduced model-based temperature gradient and its per-component contributions

3.3 Candidate estimation structures

According to the preceding developments, the two-effluent composition estimation task for the six-component system (2) can be performed using the reduced three-component model with one temperature sensor located between 25-th and 33-rd stages, with the C3 component as innovated state in a robustness-oriented GE with passive structure (Pulis et al. (2006)). To preclude unduly bottom-to-top model and measurement error propagation, no measurement in the stripping section is placed. To have a favorable balance between data assimilation and model-measurement error propagation from the measurement to distillate effluent composition estimate, a measurement should be located in the tray interval between stages 29 and 33, and not in any of the two top trays (stages 35 and 36) as shown in Figure 1. Thus, the preceding considerations lead to the following candidate estimation structure: (i) no sensor in the stripping section, (ii) one sensor in the enriching section between 29-th and 33-rd trays, and (iii) the C3 composition as innovated state. These structural conclusions are suggestive in the sense that: (i) candidate sensor location and innovated C3 compositions around the afore concluded candidates must be examined, and (ii) the conclusive structural assessment will be performed in the next section, on the basis of GE functioning. In order to verify the estimator performance, some different choices for the set of innovated states have been selected by following the considerations above: these innovated state sets will be illustrated and compared in Section 4.

4. STRUCTURE ASSESSMENT WITH ESTIMATOR FUNCTIONING

Having as point of departure the candidate structures identified in the preceding section, in this section the estimation structure for effluent composition estimation aims is assessed on the basis of the structure behavior with a robustness-oriented GE with passive structure (Pulis et al. (2006)). The role of the actual process will be played by the six-component system (2), and the GE will be implemented with the reduced three-component model (4).

4.1 Geometric estimator with passive innovation

Let us recall the adjustable-structure proportional-integral (PI) GE with passive structure (Alvarez and López (1999); Alvarez and Fernandez (2008)):

$$\begin{aligned} \dot{\hat{x}}_I &= f_I(\hat{x},\hat{u}) + \Phi_{x_I}^{-1} P(K_P(y_P - \hat{y}) + z) \\ \dot{\hat{x}}_{II} &= f_{II}(\hat{x},\hat{u}) \qquad \dot{z} = K_I(y_P - \hat{y}) \qquad \hat{y} = h(\hat{x}) \end{aligned} \tag{5}$$

where $\hat{x}$, $\hat{u}$, and $\hat{y}$ are the estimates of x, u, and y, $x_I \in \mathbb{R}^{n_I}$ is the set of the innovated states, $x_{II} \in \mathbb{R}^{n-n_I}$ is the set of the non-innovated states, K_P and K_I are respectively the proportional and integral gain matrices. For this kind of estimator structures, if $x_I = [c_{s_1}^{l_1^1} \ \dots \ c_{s_1}^{l_1^{n_1}} \ \dots \ c_{s_m}^{l_m^1} \ \dots \ c_{s_m}^{l_m^{n_m}}]^T$, then K_P, K_I, Φ_{x_I}, and P assume the following form:

$$K_P = \begin{bmatrix} K_{P,s_1} & & \\ & \ddots & \\ & & K_{P,s_m} \end{bmatrix} \qquad K_I = \begin{bmatrix} K_{I,s_1} & & \\ & \ddots & \\ & & K_{I,s_m} \end{bmatrix}$$

$$\Phi_{x_I} = \left[\left. \frac{\partial \hat{T}_{s_1}}{\partial \hat{c}_{s_1}^{l_1^1}} \right|_{\hat{c}_{s_1}} \cdots \left. \frac{\partial \hat{T}_{s_1}}{\partial \hat{c}_{s_1}^{l_1^{n_1}}} \right|_{\hat{c}_{s_1}} \cdots \left. \frac{\partial \hat{T}_{s_m}}{\partial \hat{c}_{s_m}^{l_m^1}} \right|_{\hat{c}_{s_m}} \cdots \left. \frac{\partial \hat{T}_{s_m}}{\partial \hat{c}_{s_m}^{l_m^{n_m}}} \right|_{\hat{c}_{s_m}} \right] \cdot \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} \qquad P = \begin{bmatrix} 1 \ldots 1 & & \\ & \ddots & \\ & & 1 \ldots 1 \end{bmatrix}^T$$

Note that: (i) the generic composition $c_{s_i}^{l_i^j}$ is innovated only by using temperature at s_i-th stage; (ii) n_i represents the number of innovated components at s_i-th stage and the condition $\sum_{i=1}^{m} n_i = n_I$ holds; (iii) $[x_I \, x_{II} \, z]^T \in \mathbb{R}^{n+m}$; (iv) P is a matrix of 1s and 0s, where for every column $i \in \{1, \ldots, m\}$ there are n_i 1s as shown above. When the integral action state is eliminated, the proportional (P) GE is obtained.

The robust convergence aspects and its connection with the tuning of gains can be seen in Alvarez and Fernandez (2008), and here it suffices to mention that: (i) the convergence criterion is coupled with rather easy-to-apply tuning guidelines, and (ii) the tuning scheme and guidelines apply over all structures. In this way, one has the certainty that the estimator functioning results are due to the structure and not to the tuning scheme.

Next the GE tuning guidelines for the GE PI estimator with passive structure are recalled. Consider an innovated state $c_{s_i}^{l_i^j}$: then, the corresponding temperature used in order to estimate this composition is T_{s_i} and the tuning parameters are:

$$K_{P,s_i} = 2\xi_{s_i}\omega_{s_i} \qquad K_{I,s_i} = {\omega_{s_i}}^2 \tag{6}$$

where ω_{s_i} and ξ_{s_i} are respectively the characteristic frequency and the damping factor of the estimator at s_i-th stage. The characteristic frequency ω_{s_i} must be chosen between 5 and 10 times faster than ω_{o,s_i} (where ω_{o,s_i} is the natural characteristic frequency of composition at s_i-th stage). Following conventional-like filter and control behavior assessments, the estimator functioning will be measured with the IAE index and the steady-state error.

As mentioned before, the estimation task is to infer the effluent impurity compositions (i.e., C3 in the bottom and IC4 in the top). Since the C3 in the reboiler is adequately described by the model without measurement, only the results of the IC4 distillate composition estimates will be presented. Several simulations have been performed, but for sakes of brevity only one of them is reported here. To test the estimator over different structures, a column transient has been induced by some step changes at the reboiler duty ($\Delta Q = +3\%$ at $t = 2$ hrs and $\Delta Q = 0$ at $t = 8$ hrs, with respect to Q value of Table 1)

Two different measures have been employed: (i) the steady-state error (7a), and (ii) the IAE index (7b)

$$e_{i,SS1}^j \quad \text{if} \quad \Delta Q = 0 \quad \text{and} \quad e_{i,SS2}^j \quad \text{if} \quad \Delta Q = +3\% \tag{7a}$$

$$IAE(e_i^j) = \int |e_i^j| dt \tag{7b}$$

where e_i^j is the composition error for the component j at i-th stage. There are two steady-state errors, since two different steady-state conditions are present, as can be seen from Figures 4, 5, and 6. For all the structures considered, the estimator has been tuned with the tuning guidelines sketched in (6), with $\omega_{s_i} = 10\omega_{o,s_i}$ and $\xi_{s_i} = 3$ for $i = 1, \ldots, m$.

4.2 Estimation with one innovated state

On the basis of the structural analysis performed in Section 3, two single-innovated state cases have been considered: $x_I = [c_{29}^{C3}]$ and $x_I = [c_{33}^{C3}]$.

The corresponding GE behavior results are presented in Figure 4 and Table 3, showing that: (i) comparing with the reduced model behavior, in both cases the estimate error undergoes a considerable reduction by measurement injection, and (ii) the case with c_{33}^{C3}-innovation yields a slightly better behavior than with c_{29}^{C3}-innovation. This result is consistent with the conclusion reached in Section 3, as 33-th stage has the largest stage-to-stage gradient and is close to the top stage.

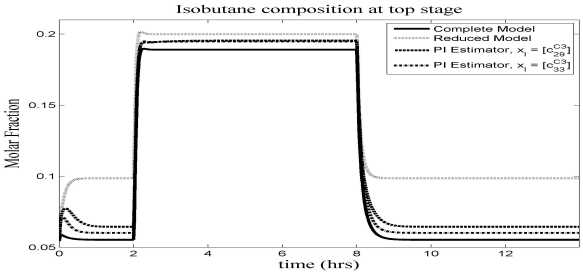

Fig. 4. IC4 distillate composition estimate with one innovated state

4.3 Estimation with two innovated states

Now, let us find out whether the joint consideration of the two previous cases leads to some estimator behavior improvement, this is $x_I = [c_{29}^{C3} \, c_{33}^{C3}]^T$.

The corresponding GE behavior results are presented in Figure 5 and Table 3, showing that there is not an appreciable improvement over the estimation structures with one innovated state discussed in the last subsection (see Figure 4).

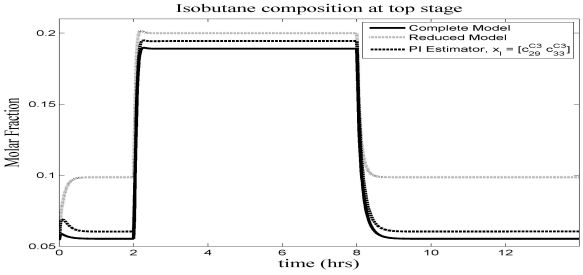

Fig. 5. IC4 distillate composition estimate with two innovated states

4.4 Estimation with three innovated states

Finally, let us investigate if the effluent estimation behavior can be improved by adding one innovated state to the two-innovated state structure presented in Subsection 4.3,

this is $x_I = [c_{29}^{C3}\ c_{31}^{C3}\ c_{33}^{C3}]^T$, with the incorporation of the innovated state c_{31}^{C3} being motivated by the fact that 29-th and 33-rd stages bracket the rich-in-information zone of the enriching section. The corresponding GE behavior results are presented in Figure 6 and Table 3, showing that there is an appreciable improvement over the two-innovated state estimation structure discussed in the last subsection (see Figure 5).

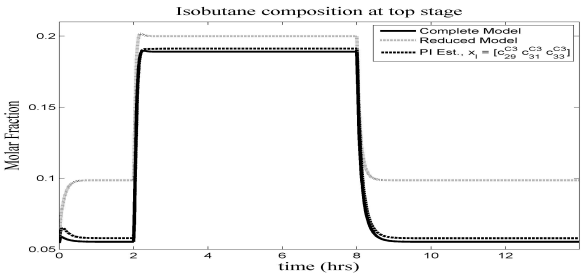

Fig. 6. IC4 distillate composition with three innovated states

Table 3. IAE values and steady-state errors (the subscript T refers to the top stage)

	$e_{T,SS1}^{IC4}$	$e_{T,SS2}^{IC4}$	$IAE(e_T^{IC4})$
Reduced model	−0.0433	−0.0109	20.1124
$x_I = [c_{29}^{C3}]$	−0.0092	−0.0064	5.9306
$x_I = [c_{33}^{C3}]$	−0.0049	−0.0058	3.8622
$x_I = [c_{29}^{C3}\ c_{33}^{C3}]^T$	−0.0052	−0.0054	3.8077
$x_I = [c_{29}^{C3}\ c_{31}^{C3}\ c_{33}^{C3}]^T$	−0.0025	−0.0022	1.7871

4.5 Concluding remarks

The behavior measures of the four estimation structures considered in this section are summarized in Table 3, showing that: the best GE estimator behavior is obtained with the three-innovated state structure, followed by the two-innovated state structure, and by the two single-innovated state structures. It must be pointed out that the steady-state estimation error is smaller than 1% and therefore comparable with typical measurement errors. These results are in agreement with the a priori structural assessments drawn in Section 3. The IC4 distillate composition estimation task can be effectively performed using: (i) a three-component reduced model, (ii) one or more sensors located between stages 29 and 33 in the enriching section, and (iii) passive innovation for component C3.

5. CONCLUSIONS

The problem of jointly designing the estimation structure and algorithm to infer an effluent composition for a six-component distillation column with temperature measurement option has been resolved in a tractable manner within a GE design framework in the light of the staged column system characteristics. The design focused on structural aspects: model reduction, sensor location, and innovation mechanism. The methodology consisted of: (i) one structural analysis step that yielded a few candidate structures and (ii) a step with conclusive structural results on the basis of estimator behavior assessment. The resulting GE (with 75 to 77 nonlinear ordinary differential equations (ODEs), depending on the structure) was considerably simpler than its EKF counterpart (with 2812 ODEs) and of tuning procedure (trial-and-error or optimization for the EKF and well defined for the GE).

Currently, work is underway to apply the proposed approach to estimate the pollutant contents in the outlet streams of an actual industrial column.

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