8th International IFAC Symposium on
Dynamics and Control of Process Systems
Preprints Vol.1, June 6-8, 2007, Cancún, Mexico

Adjustable-structure design for ternary distillation columns

[(1)] Anna Pulis, [(2)] Carlos Fernandez, [(1)] Roberto Baratti, [(2)] Jesus Alvarez

[(1)] *Dipartimento di Ingegneria Chimica e dei Materiali, Università di Cagliari, Piazza D'Armi, 09123 Cagliari, Italy*
[(2)] *Departamento de Ingeniería de Procesos e Hidráulica, Universidad Autónoma Metropolitana-Iztapalapa Apdo. 55534, 09340 México, D.F., México*

Abstract: In this work, the problem of jointly designing the estimator structure and the algorithm for ternary distillation columns is addressed. In particular, the choice of the estimation structure (measurements location and innovated states set) and the design of a complete or reduced algorithm with the possibility of changing the estimation structure during the column operation are considered. The proposed estimators are tested using experimental data from a 32-stage pilot column, finding that: (i) the structural decisions play a key role in the estimator performance, regardless of the kind of estimation algorithm employed, (ii) the best estimator behavior is obtained by injecting the temperature information over a few column states, and (ii) the same functioning is obtained with geometric estimation and EKF.

Keywords: distillation column, ternary distillation, passive estimation, process estimation

1. INTRODUCTION

The lack or high costs of composition analyzers for industrial distillation columns motivates the development of estimators to on-line infer compositions on the basis of a process model and (typically two to three) temperature measurements. The estimator design involves stuctural (sensor locations and number) and algorithmic (EKF, Luenberger observers, and so on) decisions. The related state of the art can be seen elsewhere (c.f. Alvarez et al., 1999), and here it suffices to mention that: (i) by far, the EKF has been the most widely used and accepted estimation technique (Baratti et al., 1998; Oisiovici et al., 2000; Venkateswarlu et al., 2001), (ii) the structural decision has a profound effect on the estimator functioning (Alvarez et al., 2000; Lopez et al., 2004), and (iii) the choices of number and sensor locations is still an open problem, with results that are not cleary connected with the estimator algorithm design and functioning. While some studies state that only a few (two or three) temperatures should be used in order to prevent ill-conditioning by problem overparameterization, others have questioned this claim and have pointed out the importance of looking at the relationship between measurements and states of interest (c.f., Mejdell et al. 1993).

The rapid growth of the EKF dimensionality with the number of components and stages motivates the development of a unified framework to jointly address the structure and algorithm estimation designs for multicomponent distillation columns, with emphasis on the attainment of schemes with measurement structure selection criterion, suitable data assimilation schemes, and simplified algorithms. For instance, the EKF has a data assimilation mechanism with innovation injection over the entire set of model states, and the questions are whether such complete innovation mechanism is actually at play, how many temperature sensors should be used and where they should be located, and if the measurement structure should be adaptive and how this should be done. In our previous studies, the innovated/non-innovated state partition concept (Alvarez et al., 2000; Lopez et al., 2004) has been applied to ternary distillation columns (Pulis et al., 2006a), and thermodynamically interpreted (Pulis et al., 2006b), establishing the feasibility of drawing simplified estimation algorithms. Here, a further step is taken along this structure-oriented geometric framework, with emphasis on: (i) regarding the estimation structure (i.e., the innovated/non-innovated partition, number of sensors and their location) as a design degree of freedom, (ii) finding out to which extent the estimator functioning depends or not on the choice of (geometric or EKF) estimation algorithm, and (iii) exploring the feasibility of performing the data assimilation task in the light of an adaptive sensor location scheme.

In this work, the structure-algorithm estimation design problem for ternary distillation columns is addressed, with (a possible adaptive) structure that includes the measurement number and locations, the innovated/non-innovated state partition, the choices of innovated state sets per measurement. The proposed approach is illustrated and tested with experimental data drawn from a 32-stage pilot (etahnol/tert-butanol/water) column.

2. ESTIMATION PROBLEM

Consider a continuous *N*-stage ternary distillation column with, feed rate F at composition c_F, distillate (*D*) and bottoms (*B*) at composition c_D or c_B, heat load *Q* (proportional to vapor flow rate *V*), and reflux flow rate (*R*). Under standard assumptions (constant heat of vaporization, holdup in quasi-steady state regime, linear pressure drop, and vapor-liquid equilibrium at each stage), the column dynamics are described by the following equations (Skogestad et al., 1997, Baratti et al., 1998):

• *Stripping section* ($1 \le i \le n_F$, $k = 1, 2$)

$$\dot{c}_i^k = [(R + F)\,\Delta^+ c_i^k - V\Delta^- \nu_i^k(c_i^1, c_i^2)]/\eta^{-1}(R + F) \quad (1a)$$

• *Feed tray* ($i = n_F$ $k = 1, 2$)

$$\dot{c}_{n_F}^k = [R\Delta^+ c_{n_F}^k - V\Delta^- \nu_i^k\,(c_{n_F}^1, c_{n_F}^2) + F(c_F^k - c_{n_F}^k)]/\eta^{-1}(R + F) \quad (1b)$$

• *Enriching section* ($n_F + 1 \le i \le N-1$, $k = 1, 2$)

$$\dot{c}_i^k = [R\Delta^+ c_i^k - V\Delta^- \nu_i^k(c_i^1, c_i^2)]/\eta^{-1}(R) \quad (1c)$$

• *Top Tray* ($i = N$, $k = 1, 2$)

$$\dot{c}_N^k = [R\Delta^+ c_N^k - V\Delta^- \nu_i^k\,(c_N^1, c_N^2)]/\eta^{-1}(R) \quad (1d)$$

• *Temperature measurements*

$$y_s = T_s = \beta(c_s^1, c_s^2),\ s \in [1, n_F - 1] \quad (2a)$$

$$y_e = T_e = \beta(c_e^1, c_e^2),\ e \in [n_F + 1, N] \quad (2b)$$

where ($k = 1, 2$)

$$c_i^1 + c_i^2 + c_i^3 = 1, \quad \Delta^+ c_i^k = c_{i+1}^k - c_i^k$$

$$\Delta^- \nu_i^k(c_i^1, c_i^2) := \nu_i^k\,(c_i^1, c_i^2) - \nu_{i-1}^k\,(c_{i-1}^1, c_{i-1}^2)$$

$$\nu_1^1(c_0^1, c_0^2) = c_0^E, \quad \nu_1^2(c_0^1, c_0^2) = c_0^2$$

c_i^1 (or c_i^2) is the 1st(or 2nd) component (molar fraction) composition in the i-th stage, y_s (or y_e) is the measured value of the temperature T_s (or T_e) in the s(or e)-th stage (to be determined) of the stripping (enriching) section, ν_1 (or ν_2) is the nonlinear (liquid-vapor equilibrium) function that determines the i-th component composition in the vapor phase, β is the (bubble point) nonlinear function that sets the temperature, and η is the (tray hydraulics) function that sets the exit molar flow rate from the i-th stage.

Our *estimation problem* consists in combining distillation column engineering, non-linear estimation and error propagation analysis to jointly choose the estimation structure and algorithm. By structure we mean: (i) the number and location of the temperature sensors, (ii) the innovated/non-innovated states partition, and (iii) the innovated states per measurement. By algorithm we mean the dynamic data processor that performs the estimation task, with the Geometric and EKF estimators as test algorithms. The proposed approach is tested with experimental data and the results must be put in perspective with previous ones drawn with EKF studies.

3. ADJUSTABLE-STRUCTURE ESTIMATION

From previous studies, we know that: (i) on the basis of a local observabilty analysis (about a steady-state) of a N_c-component column needs N_c-1, adequately located, temperature measurements (Yu and Luyben, 1987), meaning that at least two measurements are needed in a ternary column, and (ii) according to the adjustable-structure geometric estimation approach (Alvarez et al., 1999, Alvarez et al., 2000), if a nonlinear system is nominally completely observable with poor observabilty (Lopez et al., 2004), a better estimator behavior can be attained by performing the measurement innovation only in a subset of states. The underlying notion of robust detectability corresponds to a coordinate-dependent form of an instantaneous observability-based definition of detectability (Fernandez, 2006). In other words, the states that are nominally but not robustly observable should be transferred to a vector of non-innovated states, and this enables a design degree of freedom to look for a suitable compromise between data assimilation and (measurement and model) error propagation. In our distillation column problem this means the possibility of choosing and adapting the data assimilation structure, and these ideas are developed next.

3. 1 Detectability structure and measures

Following the adjustable-structure geometric estimation approach (Lopez, 2004, Fernandez, 2006), let us introduce the estimation structure set

$$\Sigma_k = \Sigma_k\,(\pi_{ij}, \mathbf{x}_I, \mathbf{x}_{II}), \qquad i = 1,...,m \quad j = 1,\dots,n \quad (3)$$

where π_{ij} is the vector with the temperature measurement number (i) and locations (j) represents the number of temperature sensors (subscript i) and the sensor location (subscript j), and $\mathbf{x}_I$ (or $\mathbf{x}_{II}$) is the innovated (or not-innovated) state. For structural analysis purposes, let us recall the detectability measures introduced in Lopez (2004) and employed in previous binary (Fernadez et al., 2006) and ternary (Pulis et al., 2006a,b) distillation column studies.

Regard the state set $\{c_{i-1}^1, c_{i-1}^2, c_{i+1}^1, c_{i+1}^2\}$ associated with the i-th stage, let us consider the set of admissible candidate structures (Σ_k):

$$\Sigma_1 = \{\pi_{1j}, \mathbf{x}_I = (\hat{c}_i^1, \hat{c}_i^2)'\} \quad (4a)$$

$$\Sigma_2 = \{\pi_{1j}, \mathbf{x}_I = \hat{c}_i^1 \text{ (or } \hat{c}_i^2), \mathbf{x}_{II} = \hat{c}_i^2 \text{ (or } \hat{c}_i^1)\} \quad (4b)$$

$$\Sigma_3 = \{\pi_{1j}, \mathbf{x}_I = ((\hat{c}_i^1), (\hat{c}_i^2))\} \quad (4c)$$

and their singularity measures, or equivalently, the measurement-to-state dynamics error propagation measure

$$S_i^1 = [1/\mathrm{msv}\,\mathbf{O}(\hat{c}_i, \hat{c}_{i-1}, \hat{c}_{i+1})] \quad (5a)$$

$$S_i^2 = 1/|\beta_{c_1}(\hat{c}_i^1, \hat{c}_i^2)| \text{ or } S_i^2 = 1/|\beta_{c_2}(\hat{c}_i^1, \hat{c}_i^2)| \quad (5b)$$

$$S_i^3 = [1/\mathrm{msv}\,\mathbf{O_p}(\hat{c}_i^1, \hat{c}_i^2)] \quad (5c)$$

where msv denotes the “minimum singular value”, and **O** is the estimation matrix:

$$\mathbf{O} = \begin{bmatrix} \beta_{c_1}(\hat{c}_i) & \beta_{c_2}(\hat{c}_i) \\ \partial\phi_2(\hat{c}_i,\hat{c}_{i-1},\hat{c}_{i+1})/\partial \hat{c}_i^1 & \partial\phi_2(\hat{c}_i,\hat{c}_{i-1},\hat{c}_{i+1})/\partial \hat{c}_i^2 \end{bmatrix} \quad (6a)$$

$$\mathbf{O_p}(\hat{c}_i) = \begin{bmatrix} \beta_{c_1}(\hat{c}_i) & 0 \\ 0 & \beta_{c_2}(\hat{c}_i) \end{bmatrix} \quad (6b)$$

$$\beta_{c_i}(\hat{c}_i) = \partial_{c_i}\beta(\hat{c}_i), \quad \hat{c}_i = (\hat{c}_i^1, \hat{c}_i^2)'$$

$$\phi_2(\hat{c}_i, \hat{c}_{i-1}, \hat{c}_{i+1}) = \{\beta(\hat{c}_i), [\partial_{c_i}\beta(\hat{c}_i)]f_i(\hat{c}_i, \hat{c}_{i-1}, \hat{c}_{i+1})\}$$

In a way that resembles the choice of a well-conditioned matrix via SVD (Lau et al., 1985), the sensitivity measure enables the assessment of the maximum and the least gain for each column-stage. Following previous results (Pulis et al., 2006a), a large singularity measure of the interactive estimation matrix, equation (6a), suggests the employment of the following single-innovated state estimation structure (Σ_2) for the first component in order to draw a better compromise between information injection versus measurement-modelling error propagation.

Additional information on the choice of the estimation structure can be found analyzing the behavior of the innovated (or non- innovated) states and the dynamic parameter (λ_i^{II}) in the equations (7a,b) [or equations (7c,d)]

$$\lambda_i^{II} = -(\lambda_i^n + \tilde{\lambda}_i^I), \quad \lambda_i^n = \partial f_i^2/\partial c_i^2 \quad (7a)$$

$$\lambda_i^I = (\partial f_i^2/\partial c_i^1)(\partial c_i^1/\partial c_i^2), \quad \partial c_i^1/\partial c_i^2 = \partial\beta_{c_2}/\partial\beta_{c_1} \quad (7b)$$

which stand for exponential stability margin of the non-innovated states and provides the response speed to reconstruct the states dynamic via estimator.

The same analysis can be performed for the second component. As in the previous case the single-innovated state estimation structure Σ_2 and the behavior of the non-innovated states is showed in the following equations:

$$\lambda_i^{II} = -(\lambda_i^n + \tilde{\lambda}_i^I), \quad \lambda_i^n = \partial f_i^1/\partial c_i^1 \quad (7c)$$

$$\lambda_i^I = (\partial f_i^1/\partial c_i^2)(\partial c_i^2/\partial c_i^1), \quad \partial c_i^2/\partial c_i^1 = \partial\beta_{c_1}/\partial\beta_{c_2} \quad (7d)$$

As can be seen from the equations (7) the influence of the innovated dynamic on the non-innovated depends on the ratio of the bubble point temperature derivatives. The influence of this ratio on the non-innovated dynamic suggests: (i) the composition state should not be innovated when there is a strong interaction between the innovated and non-innovated dynamics; and (ii) a robustness-oriented passive estimation structure should be used when the innovated dynamics has a weak influence on the non-innovated dynamics.

In a way that is analogous to the case of distillation column control design (Skogestad et al., 1990), to handle the strong coupling, a passive decentralized structure is considered (Σ_3) and the resulting estimator is able to satisfactory predict the output compositions (Pulis et al., 2006a) with a geometric estimator algorithm. The question is whether the same behavior can be obtained with a reduced order EKF designed according to the structural results of the geometric estimation approach. This question is addressed in the next subsections.

3.2. Geometric Estimator

The combination of the estimation structure with the GE algorithm leads to the design of an estimator with decoupled data assimilation mechanism

$$\dot{\hat{c}}_i^E = f_i^E(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T) + [1/\beta_{c_E}(\hat{c}_i^E, \hat{c}_i^T)]\{w_E + 2\zeta_E\omega_E[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)]\} \quad (8a)$$

$$\dot{\hat{c}}_i^T = f_i^T(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T) + [1/\beta_{c_T}(\hat{c}_i^E, \hat{c}_i^T)]\{w_E + 2\zeta_T\omega_T[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)]\} \quad (8b)$$

$$\dot{\hat{c}}_i^k = f_i^k(\hat{c}_j^E, \hat{c}_j^T, \hat{c}_{j-1}^E, \hat{c}_{j-1}^T, \hat{c}_{j+1}^E, \hat{c}_{j+1}^T), \quad j \neq i, j \in [1, N]$$

$$\dot{w}_E = \omega_E^2[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)], \quad \dot{w}_T = \omega_T^2[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)]$$

where ω_E , ω_T , ζ_E , ζ_T are the tuning parameters. The application of the GE tuning guidelines (Lopez, 2000; Fernandez, 2006) yielded;

$\omega_E = \omega_T = 0.03 \text{ min}^{-1}$, $\zeta_E = \zeta_T = 1.5$

3.3 Extented Kalman Filter

The application of the EKF technique to the innovated column subsystem yields the geometric EKF (GEKF):

$$\dot{\hat{c}}_i^E = f_i^E(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T) + [(\beta_{c_E}(\hat{c}_i^E, \hat{c}_i^T)\sigma_{11})/r]\{[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)]\} \quad (9a)$$

$$\dot{\hat{c}}_i^T = f_i^T(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T) + [(\beta_{c_T}(\hat{c}_i^E, \hat{c}_i^T)\sigma_{22})/r]\{[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)]\}, \quad (9b)$$

characterized by three Riccati equations:

$$\dot{\sigma}_{11} = 2(f_{c_E}^E\sigma_{11} + f_{c_T}^E\sigma_{12}) + q_{11} \quad (10a)$$

$$\dot{\sigma}_{12} = f_{c_E}^T\sigma_{11} + (f_{c_E}^E + f_{c_T}^T)\sigma_{12} + f_{c_T}^E\sigma_{22} \quad (10b)$$

$$\dot{\sigma}_{22} = 2(f_{c_E}^T\sigma_{12} + f_{c_T}^T\sigma_{22}) + q_{22} \quad (10c)$$

where $f_{c_i}^k(\hat{c}_i) = \partial_{c_i} f^k$

From a structural point of view, both the GEKF and the GE are characterized by a structure with a reduced number of equations, a diagonal model error covariance matrix, and 3 tuning parameters. The implementation and tuning of the GEKF (67 eqs.) and GE (64 eqs.) is considerably simpler than the one of the CEKF (2144 eqs.), in the understanding that the tuning of the CEKF is basically performed by trial-and-error (Venkateswarlu et al., 2001) or optimization (Baratti et al., 1995; Baratti et al. 1998) procedures.

3.4 Adjustable-structure

In the last section the possibility of designing a geometric or reduced-order EKF algorithm, on the basis of the geometric structural characterization was established, with single-sensor measurement injections in a reduced set of innovated states, with the other states being reconstructed via open-loop estimation. The estimation structure obtained can be implemented for each sensor with good data assimilation capability, or equivalently, with the lower singularity measures. This implies an algorithm with a modular construction obtained combining more single-sensor single-innovated scheme and injecting information in few column stages per temperature measurements. In particular, the application of a modular structure may be useful when the column operates with transients over large regions of its state-space. In fact, the estimation structure obtained allows us to interrupt the error propagation mechanism in those column regions where the error propagation dominates the information assimilation.

3.5 Concluding remarks

Summarizing: (i) the estimation structure was designed by combining two low order single-sensor schemes for the innovated states and an open-loop estimator for the noninnovated state, (ii) in principle, the estimation scheme should be independent of the particular estimation algorithm choice, and (iii) the possibility of adjusting the structure to efficiently perform the data assimilation task has been enabled.

4. ESTIMATOR TESTING

The experimental data used to test the performance of the estimation algorithms were obtained with an experimental 32-stage column, located at the University of Padova (Italy).

4.1 Experimental apparatus and test motion

The ternary mixture ethanol/tert-butanol/water was fractionated in the 30-tray continuous column. The column is high 10 m and is constituted by a vertical thermosiphone reboiler, a total water-cooled condenser where the overhead vapor is totally condensed and the reflux drum is open to the atmosphere. The feed (*F*) is introduced in the 8-th stage from the bottom. Temperature are measured on-line by resistance thermometers on trays 0, 4, 8, 12, 18, 22, 26, 30, and the distillate and bottom compositions were sampled every (3-5 minutes) and measured off-line by means a gas-chromatograph equipped by a resistance detector. A linear pressure drop was assumed along the column considering that bottom and top pressure equal to 814 and 760 mmHg respectively.

Several experiments were carried out, but in this work were considered those characterized by rather drastic changes for which the column moves from low to high separation with a nearly constant separation regime in the final period. From an industrial continuous column perspective these experimental runs are rather unrealistic, and resemble more transients of batch columns as well as startups or shutdowns of continuous columns. On the other hand, for the purpose at hand, the experimental runs, as we shall see, have a rather poor detectability property (due to the insensitivity of compositions of interest with respect to temperature, over an important set of stages), and this in turn signifies the testing of the proposed approach under rather severe conditions.

The experiments, whose operating conditions are presented in Table 1, are characterized by: (i) constant feed composition, (ii) a sub-cooled temperature feed ($T_F \sim 25$ °C), and (iii) a sub-cooling of the reflux stream. In the first test (Run I) the column transient was induced decreasing the vapor flow-rate while in the second test (Run II) increasing the reflux flow-rate.

TABLE 1 Operating conditions

Run	Run I	Run II
R_0 (mol/s)	0.77	0.58
F (mol/s)	1.323	1.434
$(c^E_{n_F}, c^T_{n_F})$	(0.0979, 0.0630)	(0.0835, 0.0535)
V_0 (mol/s)	1.57	1.25
ΔR	–	~ + 40%
ΔV	~ -35%	–

4.2 Thermodynamic considerations

In order to appreciate the advantages derived from the application of an estimation algorithm, in Figure 1 is shown the column response of Run I. The comparison between the model predictions and the experimental values is considerable for the distillate compositions while the deviation is marked for the bottom products. In order to improve the product estimation is important to know the relationship between temperature and compositions.

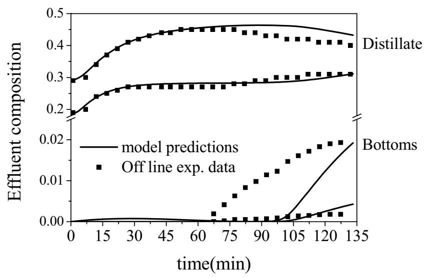

Fig. 1. Ethanol and tert-butanol model prediction (Run I).

In the previous Section was mentioned that eight temperature measurements are available, and in Figure 2 are shown the transients of the temperature and alcohol compositions stage profiles of Run I. The analysis of Figure 2 shows that temperature dynamics are faster than composition dynamics. In fact, the composition profiles are still evolving in the enriching section, while the temperatures have almost reached a steady-state condition. This says that, in a multicomponent mixture, the relationship between temperature and composition becomes rather insensitive as the compositions approach their azeotropic values, and this in turn signifies the loss of observability. Indeed, as illustrated in a previous work, when the column moves close to the azeotrope condition the temperature derivative with respect the alcohol compositions are close to zero and the singularity measure, equations (5), are higher than in the stripping section. This manifest itself as ill-conditioning of the observability matrix during the column transient, and the estimate quality. For this reason, the temperature sensor is located in the column bottom (stage 0) that represents the column region with the best data assimilation versus error propagation compromise.

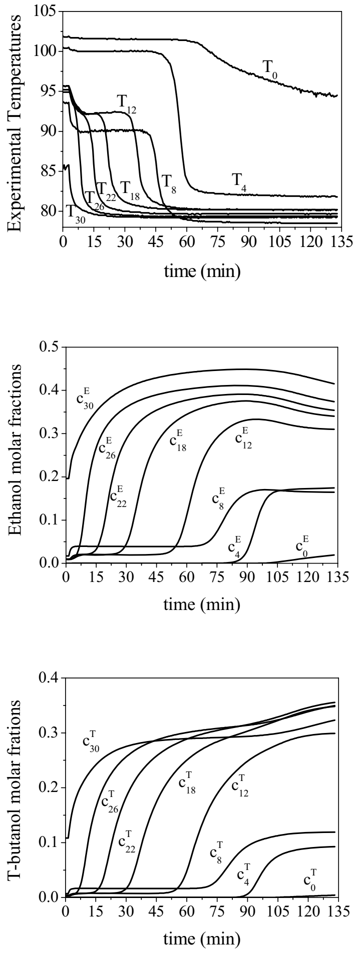

Fig. 2. Experimental temperature and simulated compositions profiles.

4.3 *Comparison between GE, GEKF and CEKF*

Here, the GE and GEKF estimators are compared with a conventional CEKF with two sensors (in the column bottom and stage 27), as it is generally done in distillation column studies. The resulting behavior is presented in Figure 3 and Figure 4, showing that basically the GE (8) and the GEKF (9) yield the same behavior. In other words, the CEKF is characterized by the combination of a complex algorithm and a full order (complete) data assimilation scheme, that is not effectively working during the process separation time. These structural issues has been tackled by means the structure-algorithm approach proposed in this work.

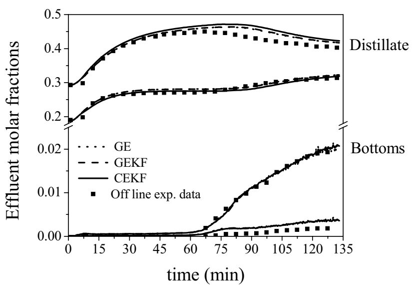

Figure 3. Comparison among GE, CEKF, CEKF estimation algorithms (Run I).

Definitely, when the structure has been adequately resolved, the data assimilation mechanism of the innovated subsystem can be designed either with GE or GEKF, simpler algorithms that efficiently perform the data assimilation task.

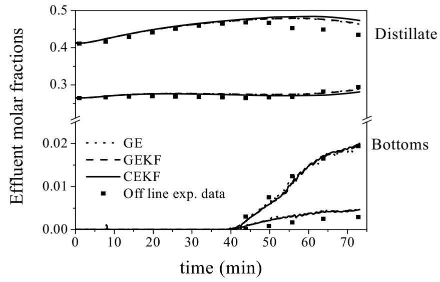

Figure 4. Comparison among GE, CEKF, CEKF estimation algorithms (Run II).

4.4 *Fixed versus adjustable structure*

Observe that good bottom composition estimates are obtained with one fixed temperature sensor located in the column bottom (stage 0). To assess the convenience of adapting the measurement location, let us analyze the possibility of extracting information content from all the available temperature measurements. As it can be seen in Figure 2, the temperature front changes with time, and this suggest us to move sensor according to the temperature wave position. The resulting adaptive adjustable-structure is obtained connecting and disconnecting two single-sensor structures, equations (8 or 9), one in the stripping section and one in the enriching section, on the basis of the evolution of the temperature wave along the column. This means changing, on-line, the selected temperature sensor, and consequently the subset of the innovated states. Specifically, the selected sensor is changed in the enriching section among the stages {12, 18, 22, 26, 30} and in the stages {0, 4} in the stripping section. The resulting estimator with an adaptive adjustable-structure is compared with a GE with one fixed temperature sensor (located in the stage 0) and the behavior is showed in Figure 5 and Figure 6. In particular, in the column considered the information content, injected in the enriching section, does not improve the composition estimation in the distillate. This is due to the thermodynamic consideration previously done, however the adaptive structure proposed could be useful in a column with better conditioned observability property, in the sense that the temperature gradients move appreciably, and where the compositions can be better inferred from the temperature measurements.

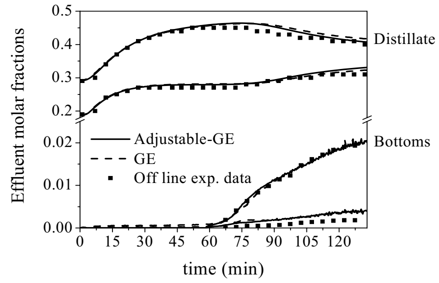

Figure 5. Comparison between a GE (with one fixed sensor) and a GE with an adjustable structure (Run I).

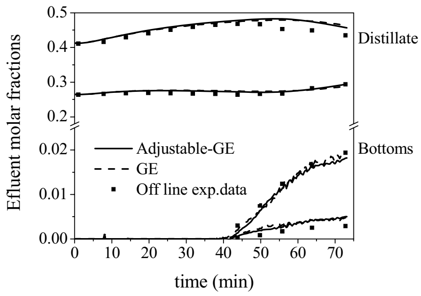

Figure 6. Comprison between a GE (with one fixed sensor) and a GE with an ajustable structure (Run II).

5. CONCLUSIONS

The structure-algorithm estimation problem for ternary distillation columns has been addressed. The choice of the (possibly adaptive) estimation structure (measurements location and innovated states set) and the design of a complete or reduced algorithm with the possibility of changing the estimation structure during the column operation were considered. The proposed approach was illustrated and tested with a 32-stage pilot column with experimental data generated by the transient response induced by rather atypical runs for a column working in continuos regime, in the understanding that these runs signify a rather difficult column estimation problem, or equivalently a severe test for any estimation algorithm. It was found that the structural-algorithm approach proposed played a key role leading to the data assimilation scheme better suited for the column considered and to a simpler algorithms that efficiently performs the data assimilation task. in the estimator performance, and the best estimator behavior is obtained by injecting the temperature information over a few column states. Provided an adequate structural decision is made, the same functioning is obtained with geometric estimation and reduced-order EKF data assimilation mechanism for the innovated subsystem, and these algorithms have considerably less equations than the ones of a conventional EKF.

Acknowledgment: The authors gratefully acknowledge Prof. Alberto Bertucco for the experimental data obtained in the pilot plant located at the University of Padova. Financial support granted by MAE is gratefully acknowledged.

REFERENCES

Alvarez, J., and Lopez, T. (1999). Robust dynamic state estimation of nonlinear plants. AIChE J., 45, 107-123.

Alvarez, J. (2000). Nonlinear State Estimation with Robust convergence. J. Process Control, 10, 59-71.

Baratti, R., Bertucco, A., Da Rold, and Morbidelli, M. (1995). Development of a composition Estimator for binary distillation columns. Applications to a Pilot Plant. Chem. Eng. Sci., 50, 1541-1550.

Baratti, R., Bertucco, A., Da Rold, and Morbidelli, M. (1998). A Composition estimator for a multicomponent columns development and experimental test on ternary mixtures. Chem. Eng. Sci., 53, 3601-3612.

Fernández, C., (2006). Estimation of binary distillation columns, PhD thesis (in Spanish), Universidad Autónoma Metropolitana, México.

Joseph, B. and Brosilow, C.B.(1978). Inferential Control of Processes: Construction of Optimal and Suboptimal Dynamic Estimators. AIChE J., 24, 485.

Lang., L. and Gilles D. (1990). Nonlinear Observers for Distillation Columns. Computers Chem. Eng., 14, 1297-1301.

Lau, H., Alvarez, J. and Jensen K.F. (1985). Synthesis of control by singular value analysis: Dynamic measures of sensitivity and interaction, AIChE J., 31(3), 427-439.

Lopez, T. (2000). Estimation and nonlinear control of continous copolymer reactors, PhD thesis (in Spanish), Universidad Autónoma Metropolitana, México.

Lopez, T. and Alvarez, J. (2004). On the effect of the estimation structure in the functioning of a nonlinear copolymer reactor estimator. J. Proc. Control 14, 99-109.

Mejdell, T. and Skogestad, S. (1993). Output Estimation Using Multiple Secondary Mesurements: High-Purity Distillation. Proc. Syst. Eng., 39, No 10, 1641-1653.

Oisiovici, R.M., and Cruz, S.L. (2000). State estimation of batch distillation columns using an extended Kalman filter. Chem. Eng. Sci., 55, 4667-4680.

Pulis, A., Fernadez, C., Baratti, R., Alvarez, J., (2006a). Geometric estimation of a ternary distillation column. Preprints of the IFAC conference ADCHEM 2006, vol. II, 573-578.

Pulis, A., Fernadez, C., Baratti, R., Alvarez, J., (2006b). Themodynamic diagram based estimation structure design for ternary distillation column. Preprints of the 16th Escape and 9th PSE, 21B, 1563-1568.

Quintero-Marmol, E., Luyben, W. L. and Georgakis, C. (1991). Application of an Extended Luenberger Observer to the Control of Multicomponent Batch Distillation. Ind. Eng. Chem. Res. 30(8), 1870-1880.

Skogestad, S., Lundstrom, P., Jacobsen, E.W. (1990). Selecting the Best Distillation Control Configuration. AIChE J., 36, N. 5, 753-764.

Skogestad, S. (1997). Dynamics and control of distillation columns – A critical survey. Model Identif. Control. 18, 177-217.

Venkateswarlu, C., and Kumar, J. (2006). Composition of multicomponent reactive batch distillation optimal sensor configuration. Chem. Eng. Sci. 61, 5560-5574.

Venkateswarlu, C., and Avantika, S. (2001). Optimal state estimation of multicomponent batch distillation. Chem. Eng. Sci., 56, 5771-5786.

Yu, C.C., and Luyben, W.L. (1987). Control of multicomponent distillation columns using rigorous composition estimators. I. Chem., E. Symp. Ser., No. 104, 29.