CHEMICAL ENGINEERING TRANSACTIONS
VOL. 32, 2013
A publication of AIDIC
The Italian Association of Chemical Engineering
Online at: www.aidic.it/cet
Chief Editors: Sauro Pierucci, Jiří J. Klemeš

ISBN 978-88-95608-23-5; **ISSN** 1974-9791
DOI: 10.3303/CET1332330

Composition Estimator Design for Industrial Multicomponent Distillation Column

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The problem of on-line estimating on the basis of temperature measurements the distillate NC4 impurity in an industrial IC4/NC4 splitter (operating at Saras refinery at Sarroch in Italy) is addressed. The application of the adjustable model-based Geometric Estimation approach yields a dynamic data processor that adequately performs the estimation task in the light of a prescribed estimation tolerance with a scheme that is considerably simpler than the Extended Kalman Filter (EKF) employed in previous studies. The implementation of the proposed estimator with experimental data shows that distillate NC4 impurity can be inferred with an uncertainty similar to the one of off-line occasional determinations.

1. Introduction

Distillation columns are important energy-consuming industrial units where a mixture is separated into two or more key components. The related control problem consists in efficiently performing the component separation in the presence of disturbances, in the sense of purity within prescribed low and high limits, and non-wasteful control action. Due to high investment and maintenance costs as well as equipment reliability and measurement delay problems of on-line composition analyzers, more often than not an effluent composition controller cannot be implemented. This motivates the development of (first-principle or empirical) model-based composition estimators driven by temperature measurements for monitoring and control purposes.

Basically, this estimation problem has been addressed with the first-principle (mostly EKF) (Baratti et al., 1995, 1998) and (input-output) data driven (Mejdell and Skogestad, 1993; Kano et al., 2000) models. On one hand, the EKF functions rather well over an ample set of column types and operating condition, but its implementation requires a detailed first-principle model and the on-line integration of a number of ODEs that grows rapidly (quadraticaly) with the number of stages and components. On the other hand, the data driven approach does not require a first-principle model, but the implementation requires significant model identification effort using considerable experimental input-output data, and validity is restricted to the specific column and operating condition encompassed by the data.

Recently, the dimensionality problem of the model based EKF approach for multicomponent distillation column (Frau et al., 2009, 2010; Frau, 2011) has been addressed with the so called Geometric Estimation (GE) approach (Álvarez and Fernandéz, 2009). While in the EKF a complete observability is required and the model is fixed, in the GE only detectability is needed and the (possibly truncated) model is a design degree of freedom. Consequently, in multicomponent distillation column, the GE has considerably less ODEs then the EKF. The GE has been successfully implemented in binary laboratory (Fernandéz, 2007) and ternary pilot (Pulis, 2007) columns with experimental data, and tested with a six-component industrial scale column through simulations (Frau, 2011). These considerations motivate the scope of the present study: the implementation -for the first time- with industrial experimental data of a geometric estimator for a multicomponent (IC4-NC4 splitter) column.

Specifically, in this paper the problem of on-line estimating, within a prescribed uncertainty value, the distillate NC4 impurity for an industrial IC4-NC4 splitter (operating at Saras refinery at Sarroch in Italy) on the basis of temperature measurements is addressed. The estimator design includes decisions on the

Please cite this article as: Porru M., Alvarez J., Baratti R, 2013, Composition estimator design for industrial multicomponent distillation column, Chemical Engineering Transactions, 32, 1975-1980 DOI: 10.3303/CET1332330

number of modeled components, the innovated component (where the measurement information is injected) as well as on the number of sensors and their locations. The problem is addressed with a GE framework (Álvarez, 2000) for multicomponent distillation column (Frau et al., 2009, 2010; Frau 2011), with the examination of the per-component temperature gradient (Frau et al., 2009, 2010; Frau 2011), playing a key role in the estimation structure design. For applicability purposes, we are interested in an estimation algorithm with a number of first-principle equations that is considerably smaller than the ones of the EKF employed in the majority of previous multicomponent distillation column studies (Baratti et al., 1995, 1998).

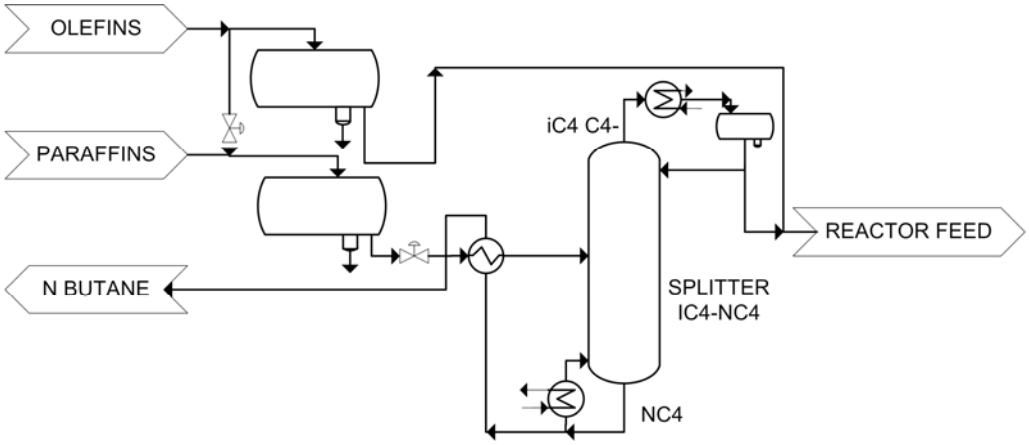

Figure 1: the splitter IC4-NC4

2. Estimation problem

2.1 IC4-NC4 splitter

Consider the industrial heptacomponent distillation column located at Saras refinery (Sarroch, Italy) and depicted in Figure 1, where iso-butane (IC4) and normal-butane (NC4) splitting occurs. Since the distillate is fed to a subsequent alkylation reactor to produce high octane gasoline, the distillate must contain mostly IC4 accompanied by a small amount, within prescribed low and high limits, of NC4. The column has 57 stages, three kettle reboilers (1st stage), total condenser (57th stage), temperature measurement at 49th stage and feed at the 33th stage made of alternately of paraffins and paraffins with olefins. The column operates switching between saturated and mixed feeds. Without restricting the approach, in this study we circumscribe ourselves to the saturated feed case. The hydrocarbons typically fed to the column are listed in Table 1, including their nominal compositions and normal boiling points. The column has a PI temperature controller that adjusts the reboiler heat injection rate on the basis of the temperature sensor in 49th stage of the enrichment section in order to maintain the heavy component (NC4) distillate molar fraction above (or below) the low (or high) limit 0.03 (or 0.07) in terms of molar fraction.

Table 1: Hydrocarbons and their nominal compositions and normal boiling points in the splitter feed

		Saturated-feed mol/mol	Mixed-feed mol/mol	Normal boiling point K
Propane	C3	0.025	0.008	231.1
I-butane	IC4	0.400	0.394	261.4
I-butene	IC4-	0.003	0.032	266.2
N-butene	NC4-	0.001	0.031	266.9
N-butane	NC4	0.569	0.467	272.7
2-butene trans	C4-TRANS	0.001	0.039	274.0
2-butene cis	C4-CIS	0.001	0.029	276.9

2.2 Experimental data

In Figure 2 are presented the industrial column data for estimator implementation: inputs feed (2.b), distillate (2.c) and reflux (2.d) flow rates as well as output temperature measurement at 49th stage (2.a). Since the feed compositions are not available for estimation, in the estimation model they are fixed at their nominal values. In the model, the three flow rates are employed to calculate the vapor and liquid streams

inside the column. The actual temperature sensor location (stage 49): must be employed to (i) test the online estimator, and (ii) ratified or rectified for structure development.

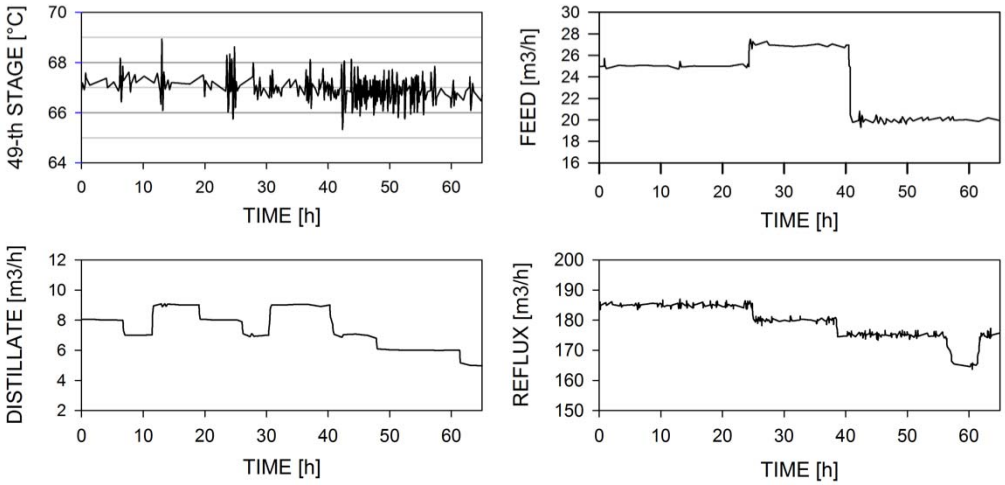

Figure 2: industrial data for estimator implementation: inputs (feed 2.b, distillate 2.c and reflux 2.d flow rates) and output (temperature measurement at 49th stage 2.a)

In Figure 3 are presented distillate NC4 experimental concentration data, with chromatographic analysis approximately every 15 minutes, in the understanding that these data will be used for estimator functioning assessment and not for estimator implementation.

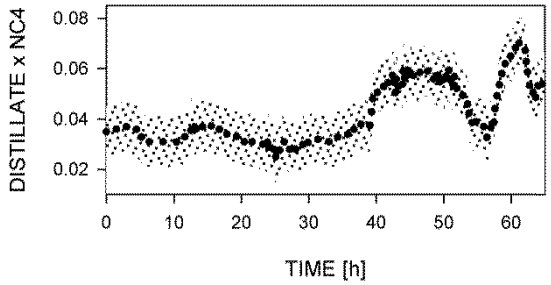

Figure 3: industrial data for estimator functioning assessment: NC4 distillate molar fraction (dotted circle) and estimation tolerance (shadow band)

2.3 Distillate composition estimation problem

Given that the control objective is to maintain the NC4 distillate composition within prescribed low (0.03) and high (0.07) limit values, the NC4 values must be estimated with an uncertainty of ± δ=0.01. Thus, our column estimation problem consist in designing: (i) the structure (number of modeled component as well as the number of sensor and their location) on the basis of the detailed column model ($N \cdot (C-1)$=342 ODEs where C (and N) is the number of components (and stages)), (ii) the on-line estimation algorithm with a simplified model (to be designed), in such a way that the estimator has considerably less ODEs than the ones of the EKF. The estimator must be implemented with the above discussed industrial experimental data (Figure 2) and assessed with the concentration data (Figure 3). The convenience of relocating the measurement and of using more than one sensor will be considered.

3. Estimator design

In this section the estimator structure and algorithm are designed according to the GE approach (Álvarez and Fernandéz, 2009) for distillation columns (Frau et al., 2009, 2010; Frau, 2011), on the basis of the per-component temperature gradient (PCTG) diagram (Frau et al., 2009, 2010; Frau, 2011) associated with steady state column operation. By structure it is meant the (possibly reduced) number of components in the estimation model, the innovated component (i.e., the one that undergoes direct innovation by measurement injection), as well as the number of sensors and their locations. By algorithm is meant the dynamic data processor that performs the on-line estimation task.

3.1 Structure design

In Figure 4 is presented the PCTG diagram associated with the nominal steady state column operation, drawn with a detailed 7-component column model, which derives from the application to the material balances for every modeled component in each stage (Baratti et al., 1995).

Based criteria to choose the estimation model structure are the following (Frau et al., 2009, 2010; Frau, 2011): (i) choose as model states (IC4 and NC4) the ones which are in greater per-section quantity, and (ii) choose as innovated component-sensor location pair (IC4-stage 43) the one in the rectifying section whose effluent is the one of interest where the innovated component exhibits the largest per-component contribution to the step-to-step temperature gradient, in such a way that its presence and change are adequately detected by the temperature measurement.

It must be point out that: (i) the actual sensor location (stage 49) is sufficiently sensitive (>1 °C in per key component basis) to set an estimator with adequate functioning (Frau et al., 2009, 2010; Frau, 2011), (ii) the best sensor location is around stage 43 (≈1.8 °C in key per component basis), and (iii) consequently, the sensor relocation from stage 49 to 43 constitutes an opportunity for the improvement of the control and monitoring schemes.

The two component (pseudo-binary) model associated with the above concluded structure, with $N(C_M\text{-}1)$ ODEs, is given by (1).

$$\dot{x} = f(x,u,d) \qquad y = h(x) \tag{1}$$

where:

$$x = [c_1^T,..., c_M^T]^T, u = [V_s], d = [F, c_F^T]^T, y = [\beta_{M\,s_i}], c_j = [c_j^{\rho_1},..., c, c_j^{\rho_{c_M}-1}],$$

$$c_F = [c_F^{\rho_1},..., c_F^{\rho_{c_M}-1}]^T, \beta_{M\,si} = \beta_M(c_{s_i}, P_{s_i}), \dim(x) = n_M = N(C_M - 1)$$

In notation above, *x, u, d* and *y* are respectively the model states, input, disturbances and output, c_i is the model vector composition at i[th] stage, c_F is the model vector feed composition and β_{Msi} is the bubble point function. c_M and *M* are respectively the number and the set of modeled components, ρ is the component set and ρ_{Mj} is the name of the j[th] modeled component, s_i is the i[th] stage, *N* is the number of stages, V_s is the vapour injection flow rate. The thermodynamics (liquid-vapour equilibrium and bubble point functions) are set with the 5-parameter Wagner equation (Raid et al., 1988).

3.2 Algorithm design

Basically, the geometric estimator is made by model (1) plus innovations, one per sensor, by measurement injection driven by the output mismatch and integration according to the expressions (2), written for the one sensor case:

$$\dot{\hat{x}}_I = f_I(\hat{x},\hat{u},\hat{d}) + \frac{1}{\beta_{c_I}}\left[K^P(y-\hat{y}) + z\right] \tag{2}$$

$$\dot{z} = K^I(y-\hat{y})$$

where: $x_I = [c_I], \beta_{c_I} = \left.\frac{\partial \beta_{s_K}}{\partial \hat{c}_I}\right|_{\hat{c}_{sk}}$.

$\hat{x},\hat{u},\hat{d}$ and $\hat{y}$ are the estimates of *x,u,d* and *y*. c_I is the innovated component at the measurement stage s_K

The proportional and integral gains K^P and K^I have been chosen according to the tuning guidelines (Álvarez and Fernandéz, 2009), which need information about the stage characteristic frequency. In case of another sensor at i[th] stage there will be another injection similar to the one of previous equation, in the i[th] stage ODE. While this estimator needs the on-line integration of $N(C_M\text{-}1)+m=58$ ODEs, the EKF needs $[N(C\text{-}1)\cdot(N(C\text{-}1)+1)]/2+N(C\text{-}1)=58{,}995$ ODEs when the detailed model is used, and $[N(C_M\text{-}1)\cdot(N(C_M\text{-}1)+1)]/2+N(C_M\text{-}1)=1{,}710$ ODEs when the pseudo-binary model (drown with the GE approach) is used. Moreover, the implementation of the GE-based model scheme with an EKF needs only $N(C_M\text{-}1)+m=58$ ODEs.

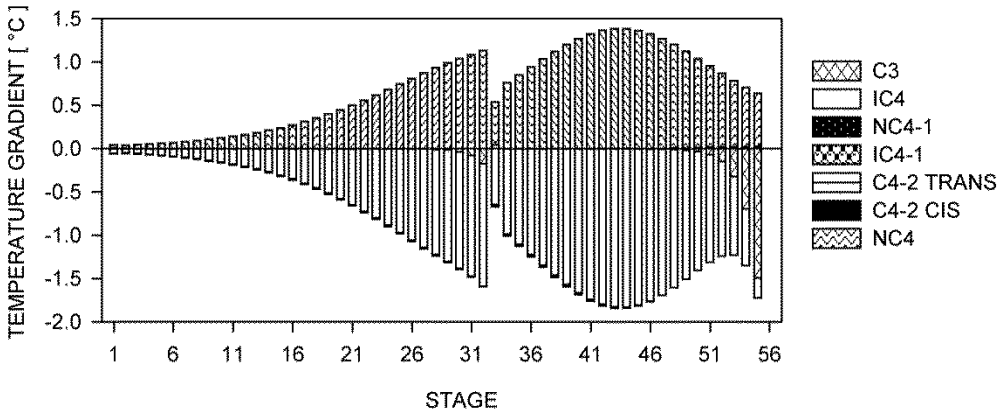

Figure 4: per-component temperature gradient (PCTG) diagram drawn with the detailed 7-component model.

4. Estimator functioning

Figure 5 shows the estimator functioning with plant temperature measurement at 49th stage. The rather good agreement between the estimated distillate NC4 molar fraction result (continuous line), and the experimental data (circle), in the light of the estimation objective represented by the tolerance shaded band demonstrates that, (i) on one hand, despite the low temperature gradient plant temperature measurements have sufficient information, and (ii) on the other hand, the system can be adequately modeled as a pseudo-column. The fact that the IC4 per-component gradient has its largest absolute value at stage 43 means that this sensor location offers the possibility for the improvement of the estimation functioning. Finally, it must be pointed out that a major number of sensor or modeled component did not offer appreciable steady state advantages.

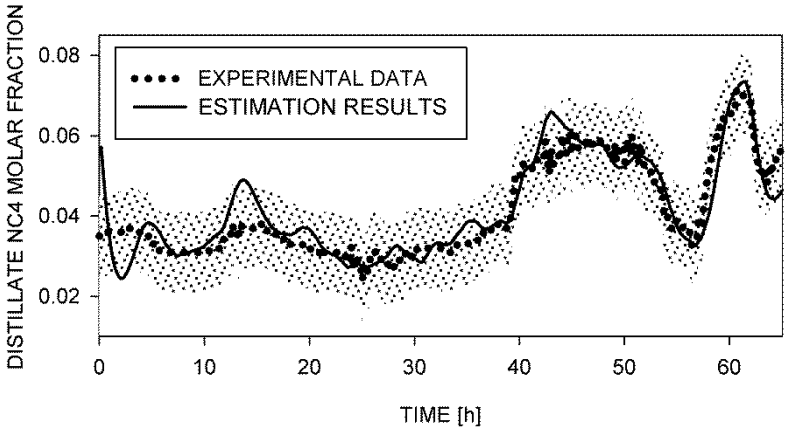

Figure 5: estimation functioning with measurement at 49th stage

5. Conclusion and future researches

The problem of online estimating, within a prescribed uncertainty band, the distillate NC4 impurity of an industrial IC4-NC4 splitter has been addressed within the GE framework, on the basis of the PCTG diagram analysis the resulting estimation algorithm is built with a two component (IC4-NC4) pseudo-binary approximation of the column and driven by one sensor between stages 43 and 50. The estimator with a sensor at stage 49 yields a satisfactory performance. According to a simulation-based analysis, the sensor location at stage 43 offers the possibility of improving the estimator behavior, and the incorporation of a second sensor does not yield a significant improvement. While the EKF has 58,995 ODEs for the complete model and 1,710 for the two component approximated model (designed with the GE approach), the proposed GE estimator has only 58 ODEs and its simplified EKF counterpart has 58 ODEs.
Work is underway to address the mixed feed case and to connect the observer and control designs.

Acknowledgement

M. Porru thankfully acknowledges SARAS refinery for the fellowship support.

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