A CRITICAL COMPARISON OF LINEAR AND NONLINEAR PROPERTY ESTIMATORS IN INFERENTIAL CONTROL

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Abstract: In this paper, a comparison of linear and nonlinear estimators with particular emphasis to the closed-loop properties of the resulting inferential control scheme is presented. The concept of closed-loop "consistency" is introduced as an effective criterion for choosing the auxiliary variables. An estimator is consistent if it guarantees low closed-loop steady-state offset in the true unmeasured controlled variables. By means of a case study of a high purity distillation column, a number of issues that can arise in inferential control are emphasized, and their implications on the closed-loop stability are discussed. It is shown that the use of some nonlinear estimators, which in general guarantee a superior precision, may be inappropriate because of the presence of zero gains and gain inversions that can lead the closed-loop system to instability. Moreover, in multi-input multi-output (MIMO) systems it is possible that the estimator requires the auxiliary variables to reach values that are not reachable by the actual plant.

Keywords: inferential control, nonlinear estimators, partial least squares, consistency, steady-state offset.

1. INTRODUCTION

In the process industries it is common to adopt property estimators as a replacement to on-line analyzers, which are very expensive (or not available for some properties) and require significant maintenance work. From a control point a view, on-line analyzers suffer from relatively large time delays which can make the control task difficult. Indeed, a common alternative is to use a number of auxiliary measurements (such as temperatures, pressures, etc.) to infer the product properties, thus building an inferential control scheme. The issue of measurement selection is of crucial importance for the effectiveness of an estimator, and it has been the subject of extensive research in the chemical engineering community (Joseph and Brosilow, 1978; Mejdell and Skogestad, 1991; Morari and Stephanopoulos, 1980; Yu and Luyben, 1987). In particular when multiple auxiliary variables are used, problems related to potential collinearity of these variables need to be addressed. Linear multivariate regression techniques, like Partial Least-Squares regression (PLS) can be used to overcome these problems and improve the robustness of the estimators as suggested by Mejdell and Skogestad (1991).

Often property estimators are based on linear relations between the auxiliary variables and the property to be estimated. However, several nonlinear regression methods like Neural Networks and nonlinear PLS (Baffi *et al.*, 1999; Qin and McAvoy, 1992; Wold *et al.*, 1989) have been proposed, and there is therefore a natural interest in evaluating their applicability for building nonlinear property estimators.

The common approach is to evaluate the estimator effectiveness in terms of precision in fitting (training and validation) data, without addressing the implica-

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tions of the estimator characteristics on the resulting inferential control scheme. To address this problem, Pannocchia and Brambilla (2003) introduced a new concept of closed-loop "consistency", which allows one to choose the most appropriate auxiliary variables for designing an effective estimator to be used in an inferential control scheme. The estimator consistency is not necessarily related to the estimator precision, that is an estimator that is precise in fitting the data may be inappropriate for inferential control because it may lead to undesired steady-state offset. In the present paper this concept is revisited in a context of nonlinear estimators, and a critical evaluation of linear and nonlinear estimators in terms of closed-loop properties is presented.

2. REVIEW OF REGRESSION METHODS

PLS has been recognized as a powerful linear regression technique in many areas of process system engineering (MacGregor *et al.*, 1994; Mejdell and Skogestad, 1991; Qin and Dunia, 2000; Wise and Gallagher, 1996). Among the large number of nonlinear regression methods, the attention of this paper is focused on nonlinear modifications of the PLS algorithm. In particular, the quadratic PLS algorithm (Baffi *et al.*, 1999) is briefly reviewed in this section.

Given a vector $Y \in \mathbb{R}^n$ of measured values of the property of interest and the corresponding values of the m auxiliary variables arranged row-wise in a matrix $X \in \mathbb{R}^{n\times m}$ (both centered around reference values y^s and x^s, respectively, and scaled to unity variance), the objective of PLS is to extract a pairs of vectors called "latent variables" $t_i \in \mathbb{R}^n$ and $u_i \in \mathbb{R}^n$ related to each other as follows:

$$u_i = f(t_i) + e_i, \qquad i = 1,2,\ldots,a\,, \tag{1}$$

where $f(t_i)$ depends on the particular algorithm chosen, and e_i is the approximation error. The auxiliary variables are related to the corresponding latent variables by a linear relation, i.e. :

$$t_i = X r_i, \qquad i = 1,2,\ldots,a\,, \tag{2}$$

in which $r_i \in \mathbb{R}^m$ is a vector of appropriate coefficients. Linear PLS (Wold *et al.*, 2001) uses a linear "inner" relation $f(t_i) = b_i t_i$, while quadratic PLS (Wold *et al.*, 1989) uses the following relation:

$$f(t_i) = c_{1,i} t_i + c_{2,i} t_i^2, \qquad i = 1,2,\ldots,a\,, \tag{3}$$

in which each element of $t_i^2 \in \mathbb{R}^n$ is the squared value of the corresponding element of t_i. In the original quadratic PLS (Wold *et al.*, 1989) the coefficients $c_i = [c_{1,i},\, c_{2,i}]$ are computed by least-square regression between t_i and u_i. Baffi *et al.* (1999) proposed a different choice for c_i aimed at minimizing the regression error e_i. This is achieved by iteratively modifying the regression coefficients of r_i used to generate t_i from X. This approach is shown to be superior to the original quadratic PLS, and is chosen in the present paper.

For prediction purposes, given a vector of the m auxiliary variables (centered and scaled) $x \in \mathbb{R}^m$, one can compute the corresponding vector of x-latent variables, $t \in \mathbb{R}^{1\times a}$:

$$t = x^T R\,, \tag{4}$$

in which $R \in \mathbb{R}^{m\times a} = [r_1,\, r_2,\, \ldots,\, r_a]$. This step is followed by a quadratic "inner" relation to obtain the vector of y-latent variables, $\hat{u} \in \mathbb{R}^{1\times a}$:

$$\hat{u} = f(t) = f(x^T R)\,. \tag{5}$$

Finally, one obtains the estimate of y as:

$$\hat{y} = \hat{u} Q^T = f(x^T R) Q^T = \mathscr{H}(x)\,, \tag{6}$$

in which $Q \in \mathbb{R}^{1\times a}$ is an appropriate row vector, and $\mathscr{H}$ denotes the nonlinear relation between x and $\hat{y}$.

The estimator precision in fitting a set of data is typically expressed in terms of explained variance:

$$\mathrm{EV}(a) = 100\left(1 - \frac{\mathrm{MSE}(a)}{\mathrm{MSE}(0)}\right)\,, \tag{7}$$

in which MSE is the mean square error, defined as

$$\mathrm{MSE}(a) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i(a))^2\,, \tag{8}$$

where $\hat{y}_i(a)$ is the predicted value of y_i obtained by an estimator model using a latent variables. The explained variance (often computed on a set of data not used in training) can be used to choose the number of latent variables, a (Wold *et al.*, 2001).

3. CONSISTENCY OF LINEAR AND NONLINEAR ESTIMATORS

Consider the inferential control scheme reported in Fig. 1 in which $u \in \mathbb{R}^p$ is the manipulated variable, $y \in \mathbb{R}^p$ is controlled variable (unmeasurable), $x \in \mathbb{R}^m$ is the auxiliary variable (measurable), $\hat{y} \in \mathbb{R}^p$ is the estimate of the controlled variable, and $d \in \mathbb{R}^q$ is the disturbance. Notice that the feedback controller C operates on the estimate of the controlled variable, $\hat{y}$, and therefore it is not possible (in general) to remove steady-state offset in the unmeasured controlled variable, y. Assuming that all variables are centered (and

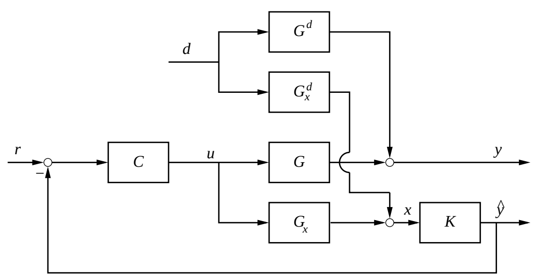

Fig. 1. Inferential control scheme

scaled) around their reference value, in a neighborhood of the origin, one can write:

$$y = Gu + G^d d \tag{9a}$$
$$x = G_x u + G_x^d d \tag{9b}$$
$$\hat{y} = \mathscr{H}(0) + Kx = Kx \,, \tag{9c}$$

in which

- $G \in \mathbb{R}^{p\times p}$ and $G_x \in \mathbb{R}^{m\times p}$ are the gain matrices from the manipulated variable to the controlled and the auxiliary variables, respectively;
- $G^d \in \mathbb{R}^{p\times q}$ and $G_x^d \in \mathbb{R}^{m\times q}$ are the gain matrices from the disturbance to the controlled and the auxiliary variables, respectively;
- $K \in \mathbb{R}^{p\times m}$ is the Jacobian of $\mathscr{H}$ evaluated at the origin, i.e.

$$K_{i,j} = \left.\frac{\partial \mathscr{H}_i}{\partial x_j}\right|_{x=0} \,, \quad i = 1,\ldots,p, \quad j = 1,\ldots,m \,. \tag{10}$$

Given the setpoint r, and assuming that the controller C has integral action, at steady state one can write

$$r = \hat{y} = Kx = KG_x u + KG_x^d d \,,$$

from which the corresponding input is

$$u = (KG_x)^{-1}(r - KG_x^d d) \,.$$

The steady-state closed-loop offset can be written as

$$e_{\mathrm{CL}} = r - y = \left[I - G\,(KG_x)^{-1}\right] r + \left[G\,(KG_x)^{-1} KG_x^d - G^d\right] d \,. \tag{11}$$

For convenience of notation, let ε_r and ε_d be the following matrices

$$\varepsilon_r = I - G\,(KG_x)^{-1} \tag{12a}$$
$$\varepsilon_d = G\,(KG_x)^{-1} KG_x^d - G^d \,. \tag{12b}$$

The steady-state offset is given by $e_{\mathrm{CL}} = \varepsilon_r r + \varepsilon_d d$. Thus, ε_r and ε_d can be regarded as the gain matrices from the setpoint reference and the disturbance, respectively, to the steady-state offset. Therefore, in order for an inferential control scheme to guarantee low closed-loop offset, it is desirable to keep some norm of ε_r and ε_d as low as possible. Such a property of an estimator is referred to as “consistency”. It is important to recognize that consistency is not necessarily related to the estimator precision. As an example, consider the case in which the number of auxiliary variables equals the number of controlled variables, i.e. $m = p$. In such case, the matrix K is square and, hence, ε_d is independent of K, which implies that consistency for disturbance rejection is independent of the estimator model. In fact, in the presence of a disturbance the control system adjusts the p manipulated variables to bring the p auxiliary variables to the corresponding nominal reference value. Hence, in such cases the estimator consistency is only dependent on the choice of the auxiliary variables, and it is often the case that auxiliary variables that are not the most precise are indeed the most appropriate for guaranteeing low closed-loop offset.

4. CASE STUDY

As a case study we choose a high-purity two-product six-component distillation column, simulated by means of Aspen Plus 11.1. For space limitations, only a brief description of the case study is presented in this paper. More details can be found in (Leoni, 2003). Nominal compositions of feed and products are reported in Table 1, and main operating parameters in nominal conditions are reported in Table 2. The column consists of 60 ideal stages, total condenser (stage no. 1) and Kettle reboiler, and the saturated liquid feed enters at the 32nd stage. In order to build and compare several property estimators, a training database of 61 runs is obtained by varying the main operating parameters one-by-one in a wide range, as briefly described in Table 3. The data used are from open-loop tests. The possibility of using closed-loop data (Macgregor *et al.*, 1991), that is with a temperature controller on a tray, is appropriate only if the tray temperature represents a “consistent” auxiliary variable. (Moreover, data should be also collected by varying the setpoint of this temperature controller, otherwise all data correspond to approximately the same temperature, because of the feedback controller). If this is not the case, and it is not possible to move the temperature controller to a different tray (Semino and Brambilla, 1996), it may be convenient to remove the temperature controller and collect only open-loop data.

Table 1. Nominal composition of feed and products (mole basis)

ID	Name	Feed	Top	Bottom
LLK_1	i-butane	0.05	0.111	0.000
LLK_2	2-methylpentane	0.10	0.223	0.000
LK	n-hexane	0.30	0.661	0.005
HK	2,2-dimethylpentane	0.30	0.005	0.541
HHK_1	2,3-dimethylpentane	0.15	0.000	0.272
HHK_2	2,2-dimethyleptane	0.10	0.000	0.182

Table 2. Nominal operating parameters

Parameter	ID	Unit	Value
Feed rate	F	kmol/hr	100.0
Distillate rate	D	kmol/hr	44.95
Reboiler duty	Q	MMkcal/hr	2.035
Top reflux ratio	R	–	4.99
Condenser pressure	p_{top}	atm	1.1
Reboiler pressure	p_{bot}	atm	1.4

Table 3. Training set synopsis

Case	Runs	Run ID	Range
Base	1	1	–
Varying D	10	$2 \div 11$	$(0.7 \div 1.3)D_{\mathrm{nom}}$
Varying Q	10	$12 \div 21$	$(0.65 \div 1.3)Q_{\mathrm{nom}}$
Varying F	10	$22 \div 31$	$(0.7 \div 1.3)F_{\mathrm{nom}}$
Varying feed comp.	20	$32 \div 51$	–
Varying p	10	$52 \div 61$	$(0.8 \div 1.32)p_{\mathrm{nom}}$

4.1 SISO case

First, a SISO case of top product HK mole fraction control by manipulating the distillate rate is considered. Several estimators are designed by choosing the condenser pressure and one tray temperature as auxiliary variables. One latent variable is used by each estimator. In Fig. 2 the explained variance for linear and quadratic PLS estimators is plotted *vs* the tray number whose temperature is auxiliary variable. From these

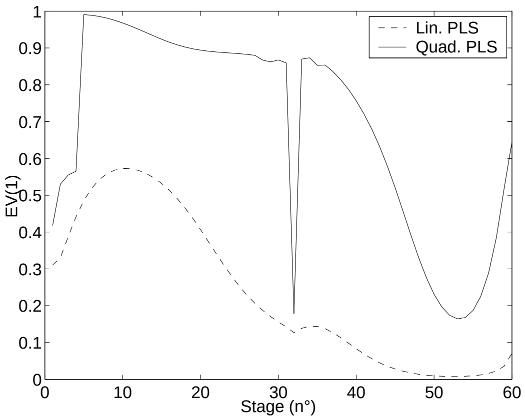

Fig. 2. Explained variance for top product estimators

results it appears that the most precise tray location is between the 8th and the 12th stage for the linear estimator, while it is between the 5th and the 10th stage for the nonlinear estimator. In Fig. 3 the most precise linear and nonlinear estimators (i.e. those with the highest explained variance) are compared in fitting the data (see also Table 3 for run IDs).

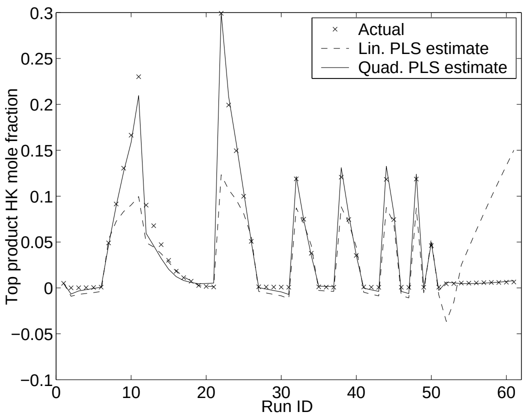

Fig. 3. Data fitting for top product estimators

From a consistency point of view, four normalized disturbances are considered:

$$d_1 = \frac{\Delta F}{F_{\mathrm{nom}}}, \quad d_2 = \frac{\Delta\left(\frac{\mathrm{LK}}{\mathrm{HK}}\right)}{\left(\frac{\mathrm{LK}}{\mathrm{HK}}\right)_{\mathrm{nom}}},$$

$$d_3 = \frac{\Delta\left(\frac{\mathrm{LLK}_1+\mathrm{LLK}_2}{\mathrm{HHK}_1+\mathrm{HHK}_2}\right)}{\left(\frac{\mathrm{LLK}_1+\mathrm{LLK}_2}{\mathrm{HHK}_1+\mathrm{HHK}_2}\right)_{\mathrm{nom}}}, \quad d_4 = \frac{\Delta P}{P_{\mathrm{nom}}}.$$

Using the training data to compute the gain matrices in (9) and numerical differentiation for computing the partial derivatives that define $K_{i,j}$ in (10), the disturbance consistency matrix ε_d is computed from (12b). Given the significant nonlinear behavior of the process, positive and negative variations of the disturbances are treated separately, thus building two consistency matrices ε_d^+ and ε_d^-, respectively. Then, the following scalar parameter is defined as a measure of closed-loop consistency for all disturbances:

$$\Phi_d = \frac{\left\| [\varepsilon_d^+,\ \varepsilon_d^-] \right\|_2}{2 \dim d}. \qquad (13)$$

In Fig. 4 the value of Φ_d for linear and nonlinear estimators is reported *vs* the tray number whose temperature is auxiliary variable. From these results, it appears

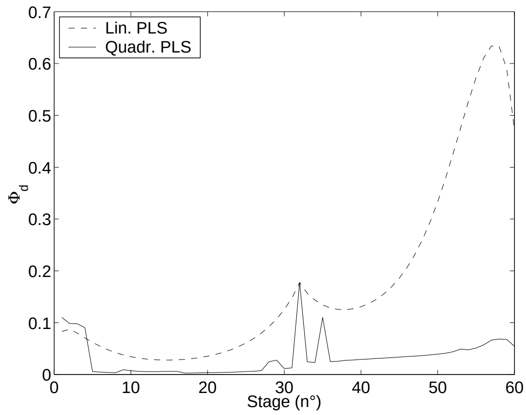

Fig. 4. Consistency parameter Φ_d for top product estimators

that the most consistent tray location is between the 12th and 18th stage for the linear estimator, while it is between the 6th to the 25th stage for the nonlinear estimator.

After this preliminary analysis, the following four estimators are compared in closed-loop rejection of the disturbances (using the Aspen Plus rigorous model):

- L_0: most precise linear estimator.
- NL_0: most precise nonlinear estimator.
- L_d: most consistent linear estimator.
- NL_d: most consistent nonlinear estimator.

Main characteristics of these estimators are reported in Table 4. In Table 5 the closed-loop offsets obtained

Table 4. Top product estimators

Est. ID	Tray	EV(1)%	$\Phi_d \cdot 10^3$
L_0	10	57.3	34.4
NL_0	5	99.1	5.6
L_d	15	53.2	27.9
NL_d	7	98.6	4.0

with each estimator in the presence of disturbances are reported. The first row (denoted with OL) refers to the open-loop offset. From these results, it appears that the estimators designed for consistency guarantee a significantly lower steady-state offset with respect to those designed for precision. On average the nonlinear estimators guarantee a lower offset than the linear estimators, even though for some disturbances (like

Table 5. Top product open-loop and closed-loop offset (multiplied by 10^3)

Est. ID	d_1		d_2		d_3		d_4		Mean
	$+0.1$	-0.1	$+0.1$	-0.1	$+0.1$	-0.1	$+0.1$	-0.08	
OL	3.9	-94.8	3.8	-32.7	3.6	-19.0	-0.3	0.5	19.9
L_0	-1.5	1.3	-0.1	0.1	-0.7	0.7	4.9	-33.6	5.4
NL_0	-2.2	2.0	0.6	-0.7	-2.0	2.1	-0.6	2.0	1.5
L_d	-1.1	1.2	-0.3	0.4	-0.4	0.4	4.	-20.7	3.7
NL_d	-1.8	1.6	0.2	-0.2	-1.2	1.3	-0.3	1.3	1.0

d_1 and d_3) the linear estimator L_d works better than the nonlinear one NL_d.

Despite these better precision and consistency properties, nonlinear estimators can exhibit a potentially harmful behavior, which arises from a non-monotonic relation between the auxiliary variables (in this case the tray temperature) and the controlled variable. As an example, Fig. 5 shows the top product HK mole fraction estimate obtained by the nonlinear estimator using the 16th stage temperature *vs* the corresponding temperature. It is clear that in such case if the setpoint

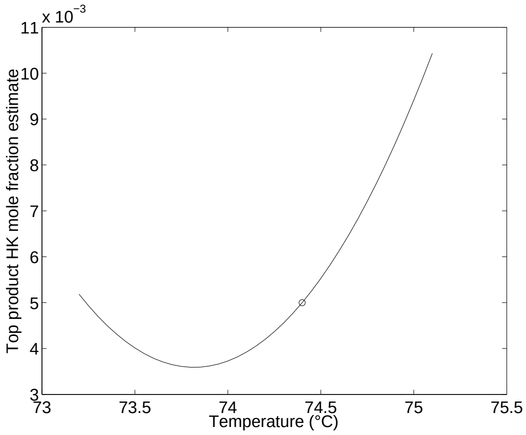

Fig. 5. Non-monotonic behavior of top product HK mole fraction estimate

is changed from 0.005 to 0.003, the control system will try to reduce the HK mole fraction estimate to the new setpoint by decreasing the distillate rate (and hence reducing the tray temperature). However, after the tray temperature reaches approximately 73.8°C, the HK mole fraction estimate increases again and the control system will further reduce the distillate rate ultimately leading to a potential closed-loop instability. Notice that this phenomenon can also occur in the presence of disturbances on the operating pressure, which move the curve in Fig. 5 vertically (up or down). This severe problem can occur with any nonlinear estimator which may have "zero gain" points and "gain inversions", while it cannot occur with linear estimators. In particular, this is likely to occurs with Neural Network models as criticized by Turner and Guiver (2002), who suggested an alternative "Bounded Derivative Network" model that is guaranteed to have monotonic relations between the auxiliary variables and the controlled variable.

Table 6. Top and bottom product estimators

Est. ID	Top product		Bottom product		Φ_d
	Tray	EV(1)%	Tray	EV(1)%	
L_0	10	57.3	50	56.6	0.126
NL_0	5	99.1	55	97.7	0.611
L_d	42	5.6	15	3.3	0.099
NL_d	13	94.2	43	83.8	0.018

4.2 MIMO case

Next, the MIMO case of top product HK and bottom product LK mole fraction control by manipulating the distillate rate and the reboiler duty is considered. For each property several estimators are designed by using the condenser pressure and one tray temperature as auxiliary variables. When addressing the problem from a consistency point of view one needs to recognize the following important observations:

- For obvious control reasons, top and bottom product estimators are not allowed to use the same tray temperature as auxiliary variable.
- Closed-loop consistency depends on both inferential control loops, so that all possible pairs of top and bottom product single temperature estimators need to be tested.
- Any estimator will be consistent for disturbances on the feed flow rate. In fact, if the feed flow rate changes and both product estimates are controlled, the steady-state temperature profile of the column will be the same as in the nominal case because both distillate rate and reboiler duty change proportionally to the feed-rate change (actually only pressure drop effects remain).

Hence, the disturbance d_1 is not considered when computing the consistency matrix ε_d and the corresponding scalar parameter Φ_d defined in (13).

Using the same rationale (best precision and best consistency) as for the SISO case, four (linear and nonlinear) estimators are designed and compared. The estimator characteristics are reported in Table 6. In Table 7 the closed-loop offsets of each product obtained by using different estimators in the presence of disturbances (not involving the operating pressure) are reported. From these results, similarly to the SISO case, it appears that the design of estimators based on consistency guarantees a lower closed-loop offset in the presence of disturbances. It is also interesting to notice that in this case the use of a nonlinear estimator model does not appear to be particularly appropriate. Furthermore, when disturbances in the operating pres-

Table 7. Top and bottom product open-loop and closed-loop offsets (multiplied by 10^3)

Est. ID	$d_2 = +0.1$		$d_2 = -0.1$		$d_3 = +0.1$		$d_3 = -0.1$		Mean	
	Top	Bottom	Top	Bottom	Top	Bottom	Top	Bottom	Top	Bottom
OL	3.8	-22.3	-37.7	2.3	3.7	-13.4	-19.0	2.1	16.1	10.0
L_0	-0.2	0.4	0.2	-0.5	-0.6	0.7	0.7	-0.6	0.4	0.6
NL_0	3.0	2.2	-0.1	1.2	-0.6	2.3	2.4	-0.8	1.5	1.6
L_d	-0.3	0.4	0.2	-0.6	-0.3	0.3	0.3	-0.3	0.3	0.4
NL_d	0.1	0.5	0.3	-0.6	-0.2	0.4	0.6	-0.3	0.3	0.4

Table 8. Estimator behavior for pressure disturbance ($P = 1.012$ atm)

Est. ID	Top			Bottom		
	T_{OL}	T_S	offset	T_{OL}	T_S	offset
L_0	68.9	72.5	-	88.7	91.1	-
NL_0	68.4	70.2	-	90.1	90.7	-
L_d	85.9	88.3	-	71.4	73.9	-
NL_d	70.7	70.3	$3.8 \cdot 10^{-3}$	86.3	86.8	$3.2 \cdot 10^{-3}$

sure are considered, both linear and nonlinear estimators may lead the closed-loop system to instability. In fact, Table 8 shows results obtained for the case of -8 % pressure change. For each estimator the open-loop tray temperature and the corresponding temperature required by the estimator to remove offset in the controlled variable estimates are reported. For all estimators, with the exception of NL_d the new “target” temperatures of the two trays cannot be reached simultaneously, and hence the control system will keep increasing the distillate rate and decreasing the reboiler duty, leading the closed-loop system to potential instability.

5. CONCLUSIONS

In this paper, a critical comparison of linear and nonlinear estimators in inferential control has been presented. The emphasis of the present work has been devoted to investigate the implications of the estimator design on inferential closed-loop systems, by revisiting the concept and the definition of “consistency” (Pannocchia and Brambilla, 2003) in the context of nonlinear estimators. It has been shown that the use of the most “consistent” auxiliary variables guarantees a lower steady-state offset than the use of the most “precise” ones, for both linear and nonlinear estimators. Moreover, severe problems that can occur in closed-loop have been discussed.

- When using some nonlinear estimators it is possible to have zero gains and gain inversions, which can make the closed loop unstable. In particular, this possibility is likely to occur when using Neural Networks (Turner and Guiver, 2002).
- In MIMO systems it is possible that, in order to remove offset, the estimator requires the auxiliary variables to reach values that cannot be reached by the actual plant. That may generate closed-loop instability. In particular, for high purity distillation columns this phenomenon can occur when disturbances in the operating pressure affect the system. Additional auxiliary variables, as the mole ratio L/V, can be used to improve the closed-loop response to such disturbances (Pastore *et al.*, 2004).

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