Composition Estimation in Dividing-Wall Columns Using Temperature Measurements

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Abstract

In this work, we propose a method to estimate the product compositions in a distillation column section based on a combination of a number of temperature measurements from different locations in the column stages.

Keywords: Kaibel Column, Thermally-coupled Distillation Column, Composition Estimation, Combination of Measurements

Introduction

The Kaibel distillation column is considered as an intensified process where can replace three conventional columns and separate a feed to 4 products. This four product divided-wall distillation column (DWC) contains fully thermally coupled sections built into a single shell. This arrangement is interesting for strongly reduced energy consumption and construction costs. The tight integration makes it challenging to control, compared to the conventional sequence of simple columns.

It is critical to have a good estimate of product compositions. Reliable and accurate measurement of product compositions is one of the important issues in distillation column control. On-line composition measurement devices are expensive and not very reliable to be used directly in closed loop control and there is usually a considerable time delay that may be a limitation to control performance. Temperature measurements are fast, inexpensive and more reliable and have been used for distillation column control in industry instead of composition analyzers. Skogestad [5] presents some benefits of using temperature loops for controlling the composition:

1. *Stabilizes the column composition profile along the column*
2. *Gives indirect level control: Reduces the disturbances on level control loops*
3. *Gives indirect composition control: Strongly reduces disturbance sensitivity*
4. *Makes the remaining composition problem less interactive and thus makes it possible to have good two-point composition control*
5. *Makes the column behave more linearly*

In multi-component system, the observed temperature at a stage is not uniquely related to the composition since different compositions may give the same temperature. So, this is the motivation to use several temperature measurements for composition estimation and then use the estimated value as setpoint for controllers. Mejdell and Skogestad [1] have suggested the Partial Least Square (PLS) method for estimating the product compositions by measuring temperatures of all trays. Figure 1 shows the process schematically.

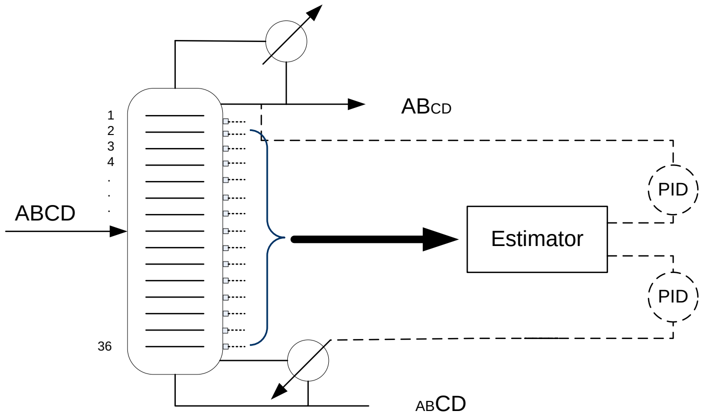


Figure 1. Schematic of the distillation process with estimator

For a specified feed component recovery, we will have a certain temperature profile in a specified feed condition. The idea is to use information from several locations in order to estimate the recovery of product composition, also for some variation in feed composition.
In this work, we propose an alternative approach for designing estimator which is to use the self optimizing control strategy (we call it “Loss method” here). This work is a continuation of the work done by Hori et al. [2]. In this work we will include noise. The number of measurements which result in one control variable depends on the number of temperature sensor locations which are put in the column during construction. This approach will be compared with the Partial Least Square (PLS) approach proposed previously ([1]).

Process Description

The Kaibel column, which is a 4-product DWC, is shown in Figure 2. The two lightest and the two heaviest products are supposed to be separated in the prefractionator and the products are separated further and drained in the main column.

The model has six degrees of freedom: boilup rate (V), reflux (L), side stream flows (S1, S2), liquid split (Rl) and vapour split (Rv), from which four will be used to keep the product compositions constant. There will remain two manipulated variables which are used as optimization variables which are used for economical purposes.

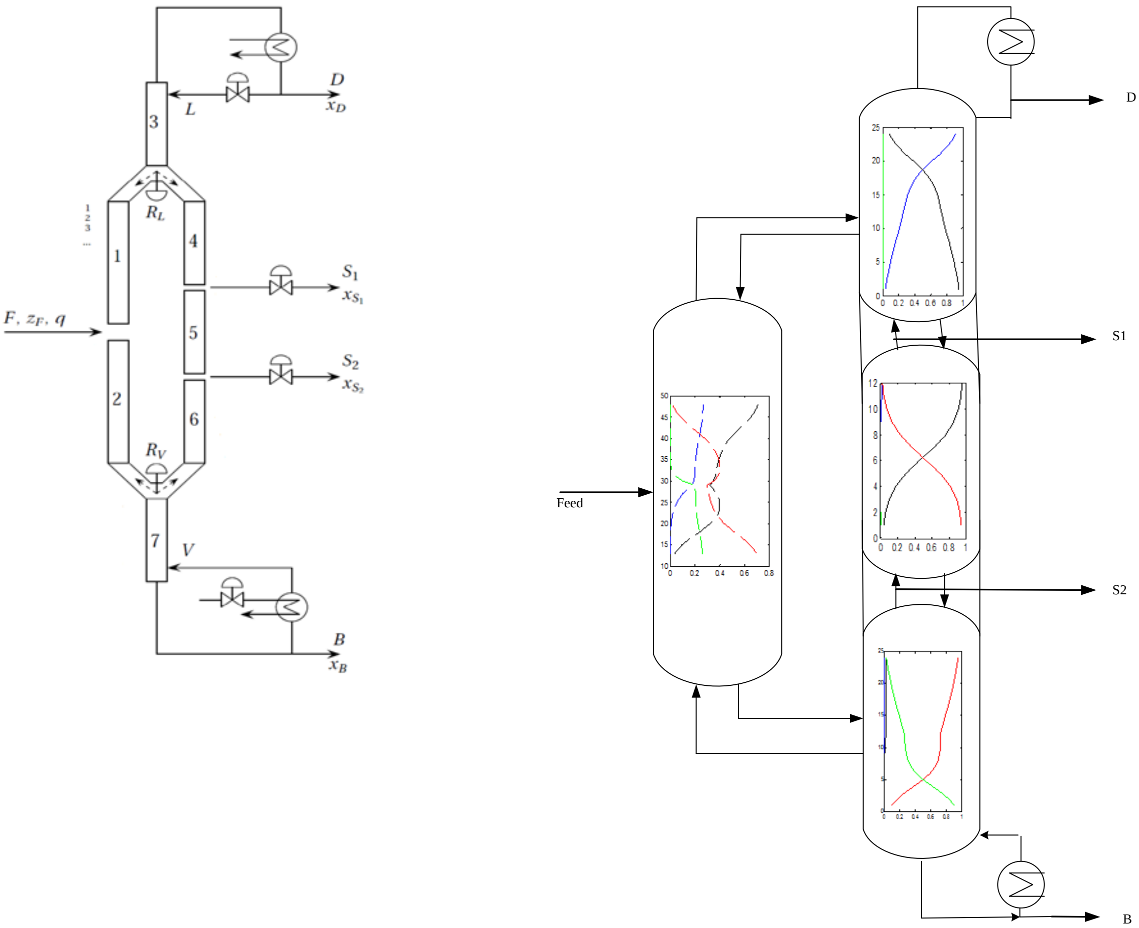


Figure 2. Schematic of a 4-product dividing wall column

The model used for this study is simulated in UNISIM. The feed stream is an equimolal mixture of Methanol, Ethanol, 1-Propanol, 1-butanol and saturated liquid. All the optimal operating points for different sets of the disturbances are found by applying an optimisation solver in MATLAB with the full non-linear model in UNISIM.

The right figure in Figure 2 shows the composition profiles in different sections of the dividing-wall column. As it is obvious, the most difficult separation is taking place in the prefractionator and the other sections are performing close to binary separation with small light or heavy impurity. Because of this, the focus of our study is on the prefractionator part.

Partial Least Square (PLS) Method

In chemometrics, partial least squares (PLS) regression has become an established tool for modelling linear relations between multivariate measurements (Martens and Næs 1989). This biased regression method is used to compress the predictor data matrix $X = [x_1, x_2, ..., x_p]$, that contains the values of p predictors for n samples, into a set of A latent variable or factor scores $T = [t_1, t_2, ..., t_A]$, where $A \leq p$. The factors t_a, $a = 1, 2, ..., A$, are determined sequentially using the nonlinear iterative partial least squares (NIPALS) algorithm [2]. The orthogonal factor scores are used to fit a set of n observations to m dependent variables $Y = [y_1, y_2, ..., y_m]$. The main attraction of the method is that it finds a parsimonious model even when the predictors are highly collinear or linearly dependent. So, the final fitting equation will be as below, with B and B_0 as optimization variables. B_0 is close to zero because of centering the data.

$$
\begin{aligned}
&Y = BX + B_0 \\
&\text{where} \quad X = \text{Temperatures} \\
&\qquad\qquad\; Y = \text{Compositions}
\end{aligned}
$$

Loss Method

The idea behind self-optimising control is to find a variable which characterize operation at the optimum, and the value of this variable at the optimum should be less sensitive to variations in disturbances than the optimal value of the remaining degrees of freedom. Thus if we close a feedback loop with this candidate variable controlled to a setpoint, we should expect that the operation will be kept closer to optimum when a disturbance occur.

Self-optimizing control is when we can achieve an acceptable loss L with constant setpoint values c, for the controlled variables (Skogestad 2000).

The optimal closed-loop estimator H is a matrix which follows the linear relationship

$$\hat{y}_1 = Hy_m \tag{1}$$

that minimizes the average and the worst case prediction error, $z = \hat{y}_1 - y_1$, where y_1 is the vector of real values for product compositions and $\hat{y}_1$ is the vector of estimated values for the product compositions. Note that the number of possible specifications is two for a two-product column, and is related to the number of available manipulative inputs, here reflux and boilup. The minimisation is done for the expected sets of disturbances (d) – namely feed flow rate, quality and compositions, and pressures of the feed and condenser –, measurement noise (n_y) and the specified product compositions. The normalized values of disturbances and noise are used in the calculations. W_d and W_n are the expected magnitudes of disturbances noise in the measurement system respectively. These come from engineering wisdom. The matrix H is the optimization variable in our method, which is equivalent to B in the PLS method.

Figure 3 shows the block-diagram of the estimation model. We need to know the linear model from inputs and disturbances to measurements and primary variables (which are product compositions). They are defined as below:

$$
G_1 = \left(\frac{\partial y_1}{\partial u}\right)_d \quad G_y = \left(\frac{\partial y}{\partial u}\right)_d
$$

$$
G_d^1 = \left(\frac{\partial y_1}{\partial d}\right)_u \quad G_d^y = \left(\frac{\partial y}{\partial d}\right)_u
$$

We also need to obtain the optimal sensitivity matrix F which is defined as

$$
F = \left(\frac{dy_{opt}}{dd}\right)
$$

which is simply obtained numerically by re-optimising the model for different disturbances.

The final task is to minimize the Frobenius norm of $H\begin{bmatrix} FW_d & W_{n^y} \end{bmatrix}$ with $HG_y = G_1$ as constraint. We will not go further into the mathematical details in this paper. The proof of this theorem is included in the coming paper.

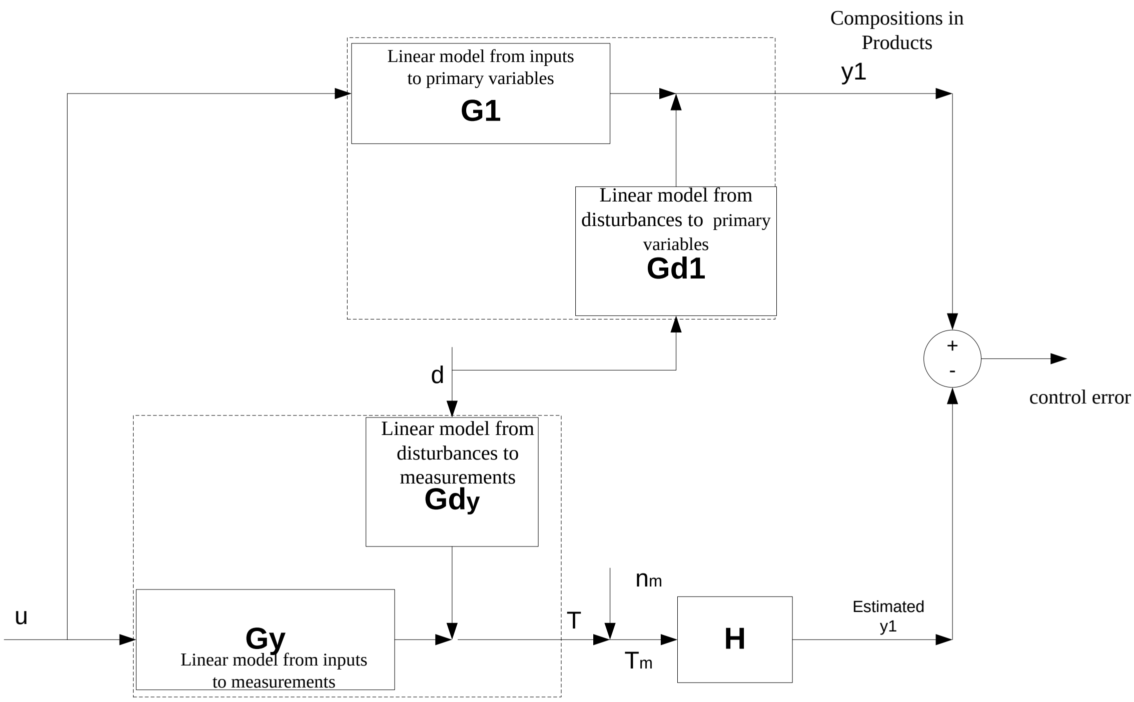


Figure 3. Block-diagram of the estimation model

Results

We assume first that we use a controller to set the manipulated variables that brings the real product compositions y_1 to the specified values $y_{1,s}$. In the steady state model this can be obtained simply by specifying prodcut compositions. The manipulated variables, here reflux and boilup, do normally not enter the estimation scheme, but these may actually be treated as measurement along with temperatures and possibly column pressure. In stead, the resulting product compositions are used. When the estimation matrix H has been calculated, the intention is to control the estimated product compositions to the specified values. Then if the estimation error is small, the real product composition will be close to the estimated ones.

Figure 3 shows a general structure for loss minimization. We can consider u to be any two variables from the process. For the sake of simplicity and because we can use the close-loop information of the system, we select the inputs to the estimation model to be equal to the product compositions, in our case

$$u = y_1 = \begin{bmatrix} x_{C_3inD} & x_{C_2inB} \end{bmatrix}$$

The matrices will be as below:

$$G^1 = I$$
$$G_d^y = F$$
$$G_d^1 = 0$$

Note the trivial G_1 and G_d^1 since we have chosen $u = y_1$.

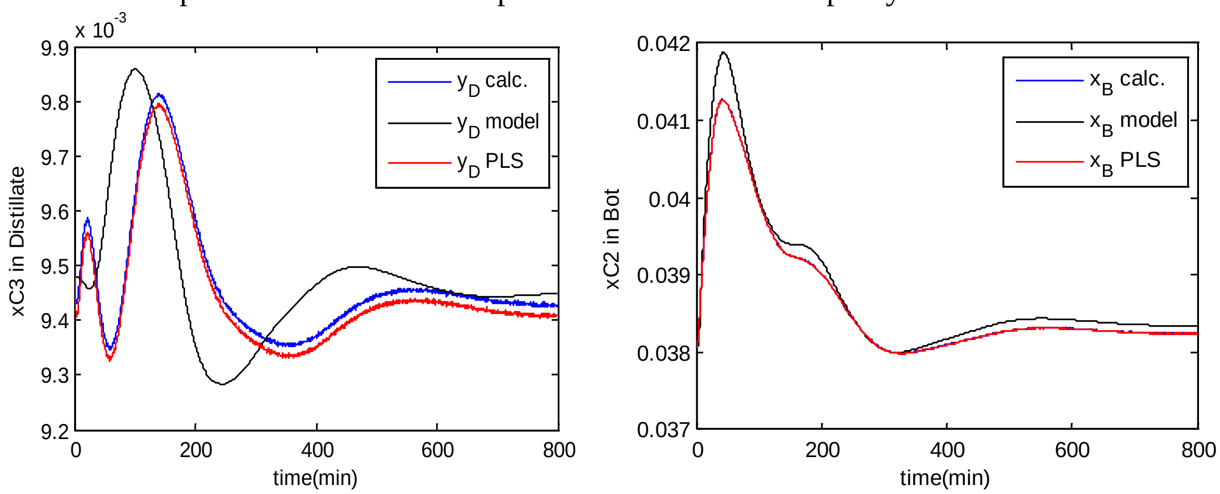
We use exactly the same information for PLS method as in our own method. X and Y in PLS method are the first and second row of Y_{all} matrix respectively.

$$Y_{all} = \begin{bmatrix} Y_1 \\ X \end{bmatrix} = \begin{bmatrix} G_1 & 0 \\ G^y & X_{opt} \end{bmatrix}$$
$$\text{where} \quad X_{opt} = \begin{bmatrix} FW_d & W_{n^y} \end{bmatrix}$$

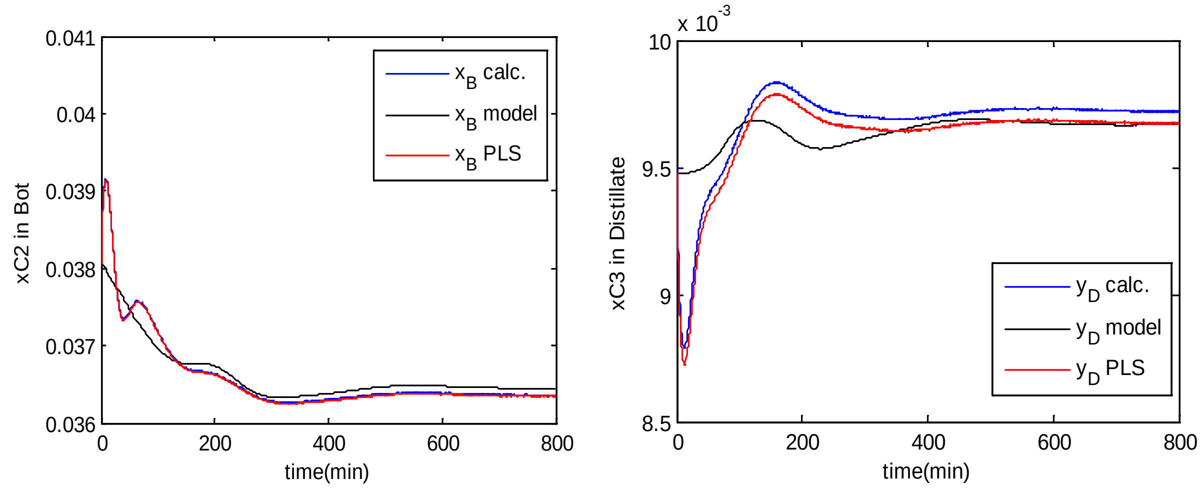
We need to know the expected "optimal variation" in x as given by the matrix $Y = X_{opt}$. Here "optimal" means that y_1 is constant (see the second column in Y_{all}). In addition, we also need to obtain G^y and G_1 from the data, which means that the data must contain "non-optimal" variations in u, and not only contain optimal data where $u = u_{opt}(d)$ - see the first column in Y_{all}.

As mentioned previously, the task of the column is to perform the sharp split of the second and third components in the feed. There will be a very small operation range for the prefractionator. This is because if we do not perform the sharp split, the impurities will end up in the side streams and the purity specifications of the side streams will be violated. So, we want to ensure to get sharp split separation in prefractionator. We need to adjust the profiles to get the split. It can be done with 1-point control, but if we want to handle feed condition changes, we will probably need to have 2-point control to be able to stay close to minimum energy consumption. In this study, we have presented the results for both cases.

Figure 4 shows the results for the case that two temperature controllers are closed and considering all the measurements. We have assumed 0.1ºC as the expected noise. The results for 1 temperature control loop are shown in Figure 5. The location of the temperature controller is found by sensitivity analysis. It was found on a tray close to the bottom end. That is why it takes more time for the top composition to stabilize. However, it can be seen that the estimated compositions follow the compositions from the model pretty well.

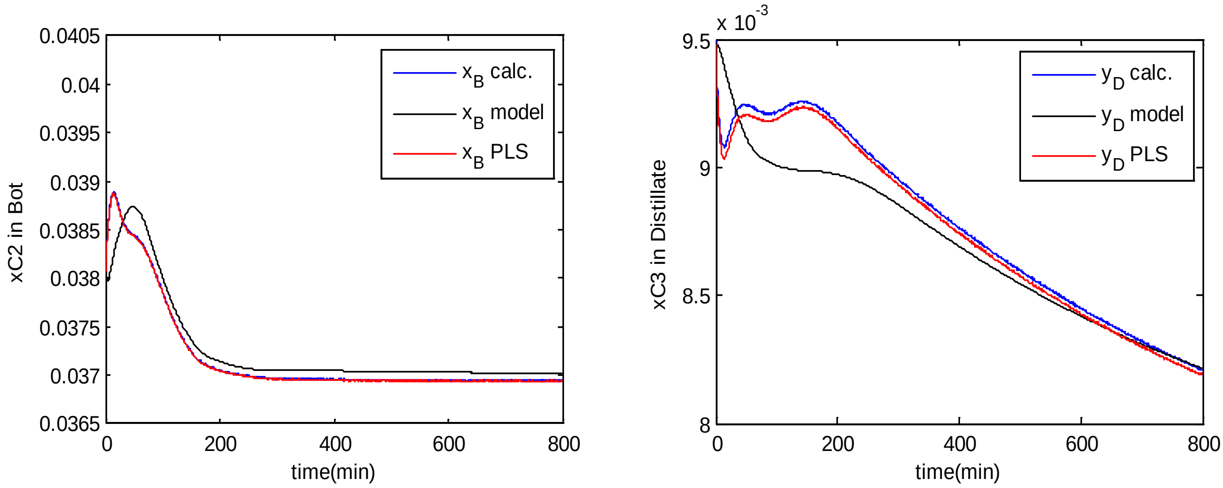


Disturbance in Feed flow rate (+5%)

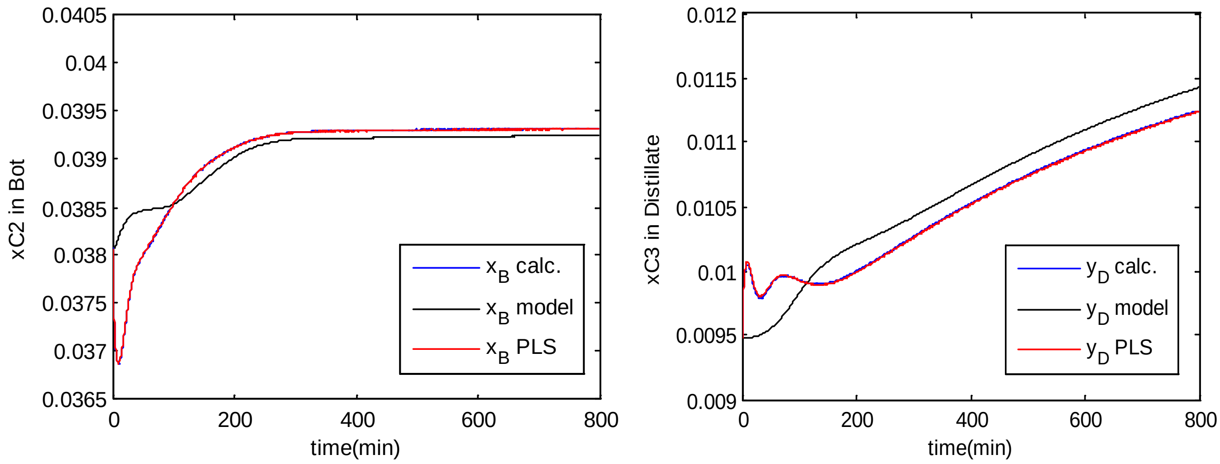


Disturbance in Feed composition z4 (-1%)

Figure 4. Estimated and model Composition values for the case with two temperature controls and with the consideration of all measurements



Disturbance in Feed quality (-1%)



Disturbance in Feed composition z1 (-1%)

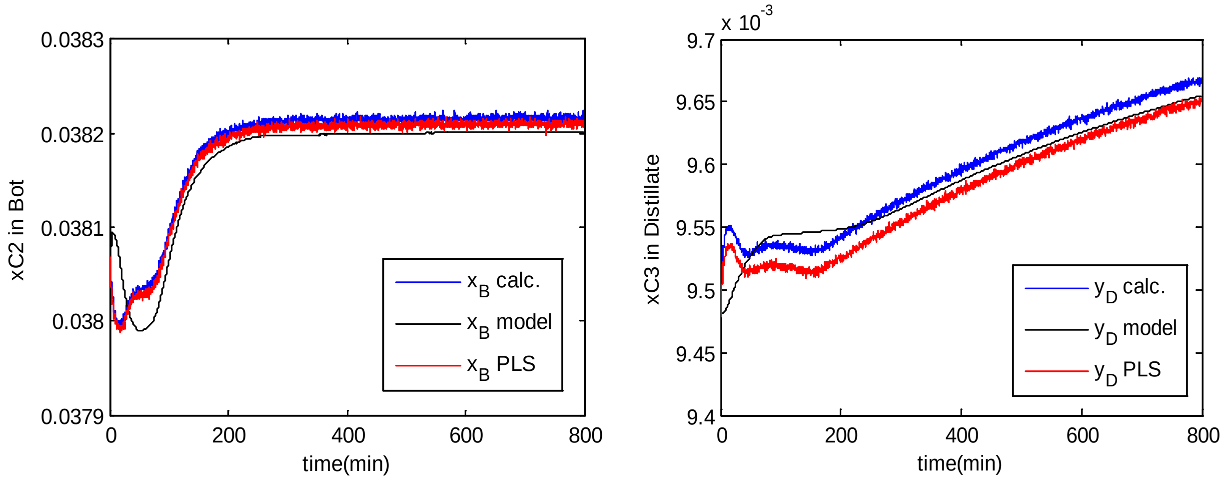
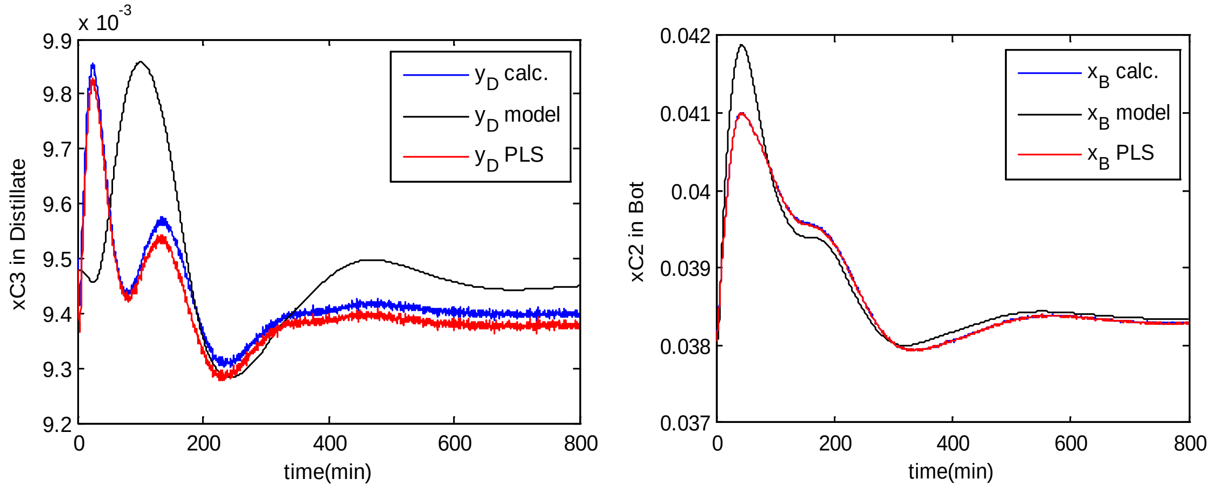


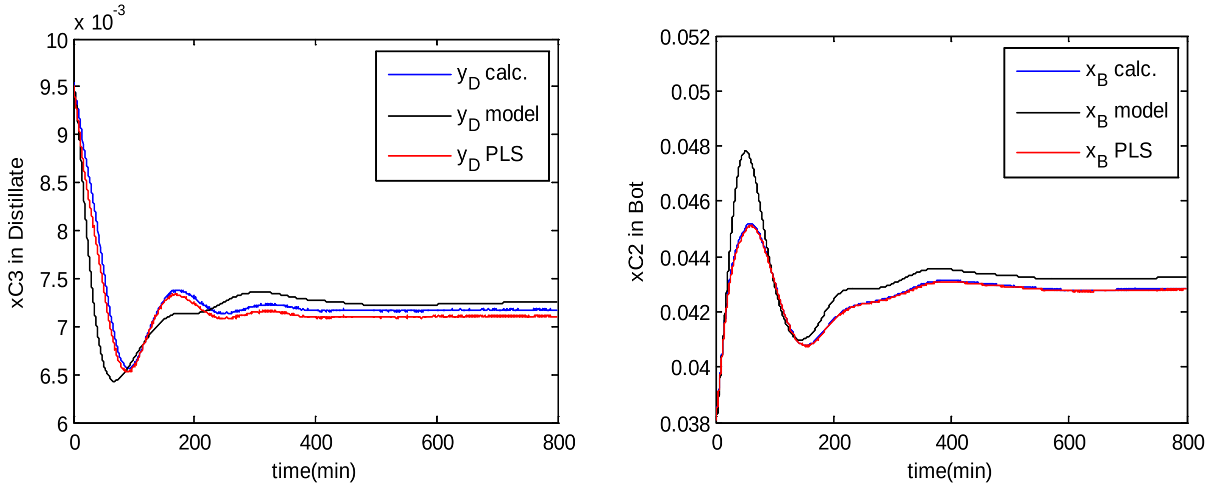
Figure 5. Estimated and model Composition values for the case with one temperature control and with the consideration of all measurements

In practical implementation, we need to consider that we do not have measurements from all the trays in the column. The more realistic case is to have temperature sensors in every 3rd or 4th tray in the column. So, Figure 6 shows the results of the estimation for two methods using data from every 4th tray in the column. The matrices in the following are the result of the calculations for PLS and Loss method. It can be seen that both matrices have the same trend in their values. It is an interesting result knowing that they have come up from two different approaches.

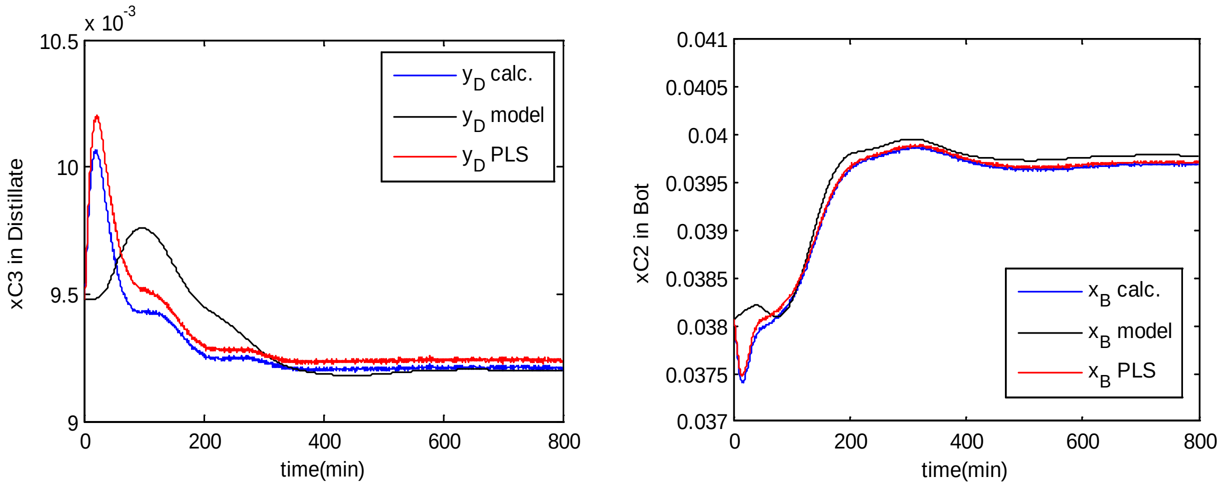
$$\beta = \begin{bmatrix} 0.0002 & 0.0013 \\ 0.0087 & -0.0041 \\ -0.006 & 0.0068 \\ -0.0051 & 0.0003 \\ 0.0077 & -0.0096 \\ -0.0034 & 0.0124 \\ -0.0016 & 0.0049 \\ 0.0026 & -0.016 \\ -0.0031 & 0.004 \end{bmatrix} \qquad H = \begin{bmatrix} 0.0004 & 0.0014 \\ 0.0081 & -0.0045 \\ -0.005 & 0.0074 \\ -0.0047 & 0.0006 \\ 0.0062 & -0.0104 \\ -0.003 & 0.0126 \\ -0.0013 & 0.0051 \\ 0.0024 & -0.0162 \\ -0.0028 & 0.0042 \end{bmatrix}$$



Disturbance in Feed flow rate (+5%)



Disturbance in Condenser Pressure (+2%)



Disturbance in Feed composition z2 (-1%)

Figure 6. Estimated and model Composition values for the case with two temperature controls and with the consideration of few measurements

Conclusions and furhter work

The results show that the new loss method and PLS method give similar results. This is interesting since the approaches are different, but the objectives are of course similar. It is important to note that the column profile should always be stabilized by a feedback. This ensures that the profiles always will be converging to a steady state, so even though a static estimator like this may be somewhat wrong in a transient it will converge to a reasonable value when approaching the steady state. This is important when the estimate shall be used as a feedback variable.

We would like to mention that this is an ongoing study, and the focus here has been on the Kaibel-column prefractionator. Our next step is to extend the procedure for the whole Kaibel column

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