A nonlinear soft sensor for quality estimation and optimal control applied in a ternary batch distillation column.

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Abstract
The present work describes the development and testing of a soft sensor based on non linear Hammerstein model which input is top Temperature and the outputs are the estimated compositions of a ternary batch distillation column. Those estimations are compared with an optimal set point computed in order to maximize the amount of distillate. A PID algorithm, optimally tuned off line by using simplified models, is used for manipulating the Reflux Ratio of the plant. Additionally the composition estimations are employed for calculating the accumulated compositions for each storage tank. Therefore a kind of split range strategy for the corresponding valves of each tank is programmed in order to accumulate each component under quality specification. The developed soft sensor made the conventional batch distillation column more efficient and easy to operate and the process control more accurate. Experiments were performed on a rigorous model developed in HYSYS PLANT validated with data of a real pilot column meanwhile all concerning to soft sensor and control policy was implemented in MATLAB. Several simulation results are presented.

Keywords: Soft-sensor Batch distillation columns Non-linear model Optimal control

1. Introduction
In recent years, industrial interest in batch distillation has increased significantly due to the need to produce low-volume/high cost materials. Achieving high quality products and improved performance of batch operations require the use of accurate process models allowing the implementation of several control methodologies. However, information on product quality and process performance is often delayed until a batch is completed. In spite of these difficulties, most of the literature on control of batch processes has focused on the development of model-based control design methods that rely on the assumption that suitable models of the system are available. That is significantly less attention has been given to the problem of how these models can be obtained from experimental data, which is the issue of identification of batch distillation processes. The rigorous model in HYSYS PLANT® is tuned to match experimental data given by Nad and Spiegel (1987). It allows accounting with enough historical plant data for applying linear and non linear identification techniques As a result a reduced

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order nonlinear model, named “Hammerstein”, relating temperature and compositions is
gained. It is used as a soft composition sensor suitable for optimal control purposes.
Hammerstein models consist of the cascade connection of a static nonlinearity and a
linear system (Ljung, 1999). The algorithm is based on Least Squares Estimation (LSE)
and Singular Value Decomposition (SVD). In addition, the linear relationship found
between temperature and reflux ratio is described by the state-space model by using a
Subspace Identification Method (namely, an N4SID method). These methods have been
successfully applied for the identification of many industrial processes (see for instance
Both simplified models (Hammerstein and N4SID) are helpful for designing the optimal
PID with its corresponding setpoint.

2. Case Study: Multicomponent Batch Distillation
The pilot plant which data are taken from Nad and Spiegel (1987) is briefly described
here. The distillation column has a 162 mm inner diameter filled with structured
packing Sulzer Mellapak 250 Y. The installed packing height was 8.0 m. The system
involves a ternary mixture of cyclohexane, n-heptane and toluene. The whole column
including reboiler and condenser has 20 theoretical plates. The initial charge is 40.07%
of cyclohexane, 39.40% of n-heptane, and 19.90% of toluene. The duration of each step
and the corresponding reflux ratio profiles are given in Jimenez et al. (2002).

The success of any identification method usually depends on the input signals being
"persistently exciting" (Ljung, 1999) to ensure that all the system modes are sufficiently
excited during the identification experiments. To overcome this problem, the rigorous
model implemented with HYSYS PLANT®, validated using the experimental data, is
excited with a sufficiently rich signal (like a PRBS) in the reflux ratio in order to
generate enough data for the identification. The simulation results were confronted with
the experimental data showing a good agreement

4. Identification Techniques and Results
Following the procedure described in sub section 4.1 it was possible to perform the
identification of a Hammerstein model. In this case, the input $u$ of the system is
temperature and the outputs $y_1, y_2$ and $y_3$ are the cyclohexane, n-heptane, and toluene
compositions, respectively. Since the sum of the three compositions is one, only $y_1$ and
$y_2$ have to be estimated. In sub-section 4.2 a brief description of N4SID methodology
adapted to this case study is presented.

4.1 LSE/SVD-based algorithm for obtaining the soft sensor
Hammerstein model consists of the cascade connection of a static (zero-memory)
nonlinearity followed by a linear time-invariant system. The method consists in making
a transformation of the nonlinear representation into an input-output model. Then, it is
linear in the new parameters, and is possible performing a regular transformation, based
on pseudo-inverse techniques, to estimate the original parameters of the linear and
nonlinear subsystems. In this paper, the methodology described in Jimenez, et al (2002)
is adapted for the estimation of the Hammerstein model.
Consider the Hammerstein model described by the following nonlinear equations

\[ y_k = \frac{b(q^{-1})}{A(q^{-1})} \sum_{i=1}^{n} c_i g_i(q^{-1}) u_{k-i} + w_k \]

\[ \sum_{i=1}^{m} b_i g_i(q^{-1}) y_{k-i} + v_k \]

where \( y_k \), \( u_k \), and \( v_k \) are the system output, input, and disturbance at time \( k \), respectively, \( g_i(\bullet) \) are nonlinear functions used to describe the nonlinear zero-memory subsystem \( N(\bullet) \), and

\[ A(q^{-1}) = 1 + a_1 q^{-1} + \cdots + a_n q^{-n}, \quad B(q^{-1}) = b_1 q^{-1} + \cdots + b_m q^{-m}, \]

with \( q^{-1} \) denoting the unit delay operator. The model is schematically depicted in Figure 1. It is assumed that the orders \( n, m, s \), and the nonlinear functions \( g_i(\bullet) \), are known, and that the goal is to estimate the parameters of the linear: \((a_1, \ldots, a_n, b_1, \ldots, b_m)\), and nonlinear: \((c_1, \ldots, c_s)\), parts from input-output data. A typical choice for the functions \( g_i(\bullet) \) is \( g_i(u_k) = u_k^i \), in which case the nonlinear subsystem is represented by a polynomial expansion. Equation (1) can be written as a difference equation of the form

\[ y_k = \sum_{j=1}^{n} a_j y_{k-j} + \sum_{i=1}^{m} \sum_{j=1}^{r} b_j c_i u_{k-j} + u_k \]

\[ u_k \]

\[ N(\bullet) \]

\[ B(q^{-1}) \]

\[ A(q^{-1}) \]

\[ v_k \]

\[ y_k \]

Figure 1: Schematic representation of a Hammerstein model

In this example, \( r = 3 \) terms were considered for the polynomial representation of the nonlinear subsystem. To select the "optimal" (in the mean square sense) order of the polynomials \( A(q^{-1}) \) and \( B(q^{-1}) \), simulations were performed for the different combinations of \( n \) and \( m \) in the range from 2 to 5, and the combination giving the minimum Mean Square Error (MSE) with the validation data was chosen as the optimal one. In this case the optimal orders were \( n = 2 \), and \( m = 3 \). The system was excited with a PRBS in the Reflux Ratio input variable. Hence the dynamic behavior of temperature in all the steps of the column was evaluated in order to choose the most sensitive one, that is top temperature which is remarked in Figure 3. The composition dynamics were considered as outputs for Hammerstein model. The resulting estimated parameters can be seen in (3) where the subscripts indicate the output channel.

\[ \hat{a}_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \hat{a}_2 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \hat{b}_1 = \begin{bmatrix} 0.7071 \\ -0.6966 \\ 0.1219 \end{bmatrix}, \quad \hat{b}_2 = \begin{bmatrix} -0.6962 \\ 0.7162 \\ -0.0477 \end{bmatrix}, \quad \hat{c}_1 = \begin{bmatrix} 0.0075 \\ -1.069 \times 10^{-4} \\ 4.6 \times 10^{-11} \end{bmatrix}, \quad \hat{c}_2 = \begin{bmatrix} 0.0277 \\ -3.698 \times 10^{-4} \\ 1.533 \times 10^{-11} \end{bmatrix} \]

4.2 Subspace-based identification methods
In recent years, considerable amount of research has been devoted to the development of identification methods that are able to deliver reliable state-space models of multivariable systems directly from input-output data. They require only a modest computational complexity without the need of iterative optimization procedures. These techniques have become collectively known as Subspace-based State-Space System Identification (4SID) Methods. The main computational tools employed by subspace methods are QR and SVD. Consider a LTI system with \( n \) inputs and \( m \) outputs that can be described by a state-space realization of the form

\[
x_{k+1} = Ax_k + Bu_k + w_k \\
y_k = Cx_k + Du_k + v_k
\]  

(4)

where \( x_k \) is the state vector, \( u_k \) is the observed input vector, \( y_k \) is the output vector, and \( w_k \) and \( v_k \) are the process noise and output measurement noise vectors respectively.

All 4SID methods involve two main steps. The first step is to perform some (weighted) projections in order to eliminate the influence of the terms depending on the inputs and the noise and then to compute estimates of the extended observability matrix and the state sequences matrix by factorizing this projection via SVD. In the second step these estimates are used to compute the system matrices \( A, B, C \) and \( D \), using mainly least squares estimation. The resulting system matrix estimates are presented in (5). The data for this methodology were the relationship between reflux ratio and top temperature is shown in Figure 3.

\[
\begin{bmatrix}
0.0009 & -0.0618 \\
0.0006 & 0.9324
\end{bmatrix}
\begin{bmatrix}
1.0009 \\
0.0006
\end{bmatrix}
\begin{bmatrix}
0.1679 \\
0.1716
\end{bmatrix}
\begin{bmatrix}
-0.1328 \\
-0.365
\end{bmatrix}
\]

(5)

5. Optimal control structure for the batch distillation column

The PID tuning was carried out off-line by using optimization techniques supported by \texttt{“fmincon” function from Matlab (Math Works Inc, 1999). The objective function was to minimize the Integral Square Error (ISE) accounting the allowed reflux ratio range and the sum of the molar factions equal to 1. Because of the time consuming in iterative
calculations when optimization technique is applied both reduced models described in the previous section were employed as a plant as shown in Figure 3. Therefore the tuning parameters were $K_1 = 56.522$, $K_2 = 1.216$, $K_3 = 3.231$, for proportional, integral and derivative modes respectively.

The control structure applied on the batch distillation is represented in Figure 4. Here, vessels P1 and P3 contain the main cuts (MC) for cyclohexane and n-heptane respectively and two off-cuts (OC), P2 and P4 with cyclohexane and n-heptane and n-heptane and toluene respectively. The off-cuts will be recycled to the reboiler at the next batch operation. Toluene product is obtained from the reboiler at the end of the batch.

The last point is to configure off-line a proper composition set point. Diwekar (1995) proposed using a combined optimization technique consisting of the maximization principle and Non Linear Programming (NLP). Two objectives were analysed, for both the idea was to maximize the amount of distillate for a given time (4.5 hours). The first one considered to achieve a molar fraction of 0.98 for cyclohexane composition at vessel P1 assuming it is the most important product to obtain. The second one proposed that both cyclohexane and n-heptane were important so composition for P1 and P3 were theoretically set to 0.98 and 0.62. Therefore the problem can be solved accounting the next relationships.
6. Results

In this section is presented how the complete structure, shown in Figure 4, can give good results to track the predefined policies given above. In Figure 5 are presented the instantaneous real composition evolutions for both cases, together with the optimal set points and the estimated compositions given by the soft sensor. Here, the real composition in P1 was 0.95851. On the other case cyclohexane and n-heptane accumulated compositions were 0.91 and 0.67 for P1 and P3 vessels. As can be seen from Figure 5 since the control point of view a good set point tracking is achieved and the soft sensor gives a good accuracy for estimating compositions. However the compositions in tanks must be corrected in order to be more closer to the specifications for accumulated composition.

![Figure 6: simulation results with Hysys and MATLAB of compositions and its corresponding reflux ratio for optimal cyclohexane (left) and optimal cyclohexane and n-heptane (right)](image)
7. Conclusions

The principal objective of this work was to show how powerful could be use a soft sensor developed by Hammerstein model for helping on implementing an optimal control problem. Additionally a combination between Hammerstein and N4SID models were helpful for obtain off-line the optimal tuning PID parameters by using the Optimization toolbox of MATLAB. The tests done supporting by two well recognized simulation software like HYSYS and MATLAB, working simultaneously thanks to a connexion protocol, allowed concluding as preliminary results that the implementation was very successfully. Then future works will be focussed on employing the soft sensor on Model Predictive Control structures.

References


