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Combining prior knowledge with data driven modeling of a batch distillation column including start-up

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Abstract

This paper presents the development of a simple model which describes the product quality and production over time of an experimental batch distillation column, including start-up. The model structure is based on a simple physical framework, which is augmented with fuzzy logic. This provides a way to use prior knowledge about the dynamics, which have a general validity, while additional information about the specific column behavior is derived from measured process data. The model framework is applicable for a wide range of columns operating under a certain control policy. The model framework for the particular column under study makes a priori assumptions about the specific behavior superfluous. In addition, a detailed description of the internal dynamics is not required, which reduces modeling effort. Three different hybrid model structures are compared; the model that uses the available sources of information most effectively can be used to simulate production including part of the start-up by applying constant quality control.

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Keywords: Dynamic modeling; Hybrid modeling; Batch distillation; Fuzzy logic

1. Introduction

Dynamic modeling for optimization and control requires models that describe the essential dynamic characteristics of the process under study. For complex nonlinear processes, a simple and effective model may be difficult to derive. The success of data driven approaches may be limited in an industrial environment where the process is subject to control and measurements are difficult to obtain, while development of a first principles model may be time consuming and expensive.

In general, three sources of information are available during model building: first principles, process data and human expertise. In many industrial situations, none of the sources provide sufficient information to build a simple model. This means that all the available information has to be combined. A good way to accomplish this is by designing hybrid models, in which first principles

are combined with data driven approaches. Some research has been done in this area (most notably by Psychogios & Ungar, 1992; Thompson & Kramer, 1994), in which artificial neural networks have been used to augment the first principles information. However, until now, little research has been presented in which fuzzy logic is used in a similar context. With respect to transparency, fuzzy logic is a very suitable technique, which makes it easier to analyze the behavior of the model.

Batch distillation is a process that can benefit from hybrid modeling. The process exhibits nonlinear behavior and has a large operating regime. In addition, the start-up of the process comprises a significant part of the operating time. For optimization and control purposes, a dynamic model should be able to describe these characteristics. A detailed model describing the internal dynamics is not required (Betlem, 2000). However, a simple overall dynamic model is difficult to derive, especially when it has to include start-up.

This paper will discuss the development of a hybrid fuzzy-first principles model for an experimental batch distillation column. The goal of the model is to describe

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the behavior of the product quality and the production over time, including an essential part of start-up. The model will be developed by using a structured modeling approach (Van Lith, Betlem & Roffel, 2002). A simplified physical model will serve as a basis and it will be augmented with fuzzy submodels, which are derived from process data. They are identified without the need for a priori assumptions about the process behavior. This way, prior knowledge is combined with information contained in the measurements. To illustrate the influence of prior knowledge, three different hybrid models will be built and compared, each with a different level of prior knowledge.

2. Process description

2.1. Start-up dynamics

Operation of conventional batch distillation can be conveniently described in three parts: (1) start-up, (2) production, and (3) shutdown period. Dependent from design and operating conditions, the start-up period can be significant compared with the production period (Skogestad & Morari, 1987). The start-up of a batch column is similar to the start-up of a continuous column. Ruiz, Cameron and Gani (1988) distinguish three stages for the start-up: discontinuous stage, semi-continuous stage and continuous stage. During the first discontinuous stage, the hydraulic variables undergo drastic changes at different instants of time. The column is heated-up from bottom to top by raising vapor and the trays are filled from top to bottom under total reflux. The end of this period coincides with the time when all tray liquid seals are established. During the second semi-continuous stage, the thermodynamic variables undergo sharp changes and the hydraulic variables reach the vicinity of their steady state values. This phase represents the most important part of the start-up operation, since it is time consuming. During the final continuous stage, the column is brought gradually at the production requirements. Due to bottom exhaustion, for batch distillation this remains a semi-steady state.

The conventional start-up policy of distillation including the semi-continuous stage have been studied experimentally by a few authors. Barolo, Guarise, Rienzi and Trotta (1994) studied a GMC policy and Ganguly and Saraf (1993) a PMC policy for a cold start-up of a sieve tray column to minimize the start-up period. The controllers were switched on, when all trays are filled. Wang, Li, Wozny and Wang (2001) developed a detailed model of a bubble-cap column including the cold start-up. The trays have a separate downcomer sealing, which is established directly after the liquid reached a tray. The model considers an empty, accumulation and equilibrium tray state. During the accu-

mulation phase a part of the liquid will flow down, when the liquid level exceeds the weir. When the temperature at a tray reaches its bubble-point, the tray is switched to the equilibrium phase. The model approximates the real progress rather well. From the figures of these three experimental studies, it can be concluded that the separation behavior during heating-up as well as tray filling-up are different. Consequently, the temperature profiles along the column at the end of the first stage are different. The behavior of the second stage depends on the controller strategy.

Simulations of start-up operations is difficult because of the complex plate hydraulics. During the first two stages of start-up, the mutual different internal tray refluxes and tray efficiencies bring about an insecure column composition profile. Wang et al. (2001), for instance, show that the temperature profile derived with their approach differ strongly from the conventional approach of Nad and Spiegel (1987). As modeling of the first stages of the start-up is rather difficult and column specific, in all simulation studies which include start-up explicitly, a so-called warm start-up is used. Usually, it is assumed that the initial compositions are equal to the charge composition (Luyben, 1971; González-Velasco, Gutiérrez-Ortiz, Castresana-Pelayo & González-Marcos, 1987; Mujtaba & Macchietto, 1992; Sørensen & Skogestad, 1996). By way of exception, Sadotomo and Miyahara (1983) determine the initial profile from the condensation of the vapor in each tray in proportion to the sensible heat of the column and the formation of the holdup. Due to the uncertainties an overall dynamic model consisting of a more qualitative dynamic framework completed with experimental data seems to be an attractive approach.

2.2. Dominant time constant

Optimization or control studies for the production period show that the tray and condenser hold-up usually can not be neglected. Robinson (1970) calculated the sub-optimal reflux trajectory for an industrial column of 47 trays. The author concluded that the hold-up could not be ignored, even though this totaled less than 4% of the initial batch charge. In several other optimization studies (Robinson, 1971; Mujtaba & Macchietto, 1996; Betlem, Krijnsen & Huijnen, 1998) the influence of the tray hold-up on the optimal control policy is determined. Betlem (2000) proved that under constant quality or constant top temperature control policy a simplified model can be applied. In that case the column behavior can be described by a dominant first-order behavior. This is comparable with the behavior of continuous columns, which has been worked out by several authors in different ways. A survey has been published by Skogestad and Morari (1987). In case of batch distillation, after start-up, the quality controller

enforces the composition profile in the column to maintain a similar shape with the bottom and top composition being pinch points. It can be proven that for a remaining similar shape a stationary dominant time constant will be obtained. Because no wave propagation of the composition profile occurs at constant quality, this result also agrees with the nonlinear wave theory (Hwang, 1991).

2.3. Experimental setup

The process involves a pilot plant batch distillation column with 21 bubble-cap trays with an internal diameter of 76 mm and a Murphee vapor tray efficiency of about 53%. The only manipulated variable is the reflux fraction R^* . The heat supply E is constant during a batch run. The maximum exhaustion time is about 4 h and the dominant time constant is about 25 min (Betlem, 2000). Start-up of a batch requires about 20–30 min, while a typical batch run for a single cut takes about 3 h. This means that start-up comprises a significant part of the batch run. A simplified diagram of the column setup is given in Fig. 1.

Measurements of five batch runs with constant quality control were available. These involve the separation of ethanol and 1-propanol for different feed stocks and equal product qualities. The data result from production runs of optimization studies. In these studies it is assumed that separations under constant quality control are almost equivalent to dynamic optimal control if the exhaustion of the bottom is kept limited (Betlem et al., 1998). The data series include a part of the start-up and end when the optimal exhaustion has been satisfied. The following measurements were available:

- distillate product quality x_{n+1} ;
- reflux fraction R^* ;

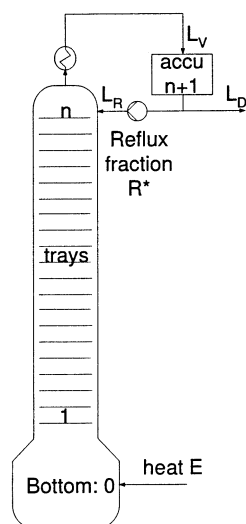


Fig. 1. Experimental batch distillation setup.

Table 1
Initial conditions for the batch distillation column

Run number	$M_{col,0}$ (mol)	$x_{col,0}$ (–)	$x_{n+1,sp}^0$
ID1	201	0.403	0.986
ID2	194	0.499	0.986
ID3	200	0.603	0.986
VAL1	193	0.410	0.986
VAL2	187	0.490	0.986

- vapor flow after condensation L_V .

Table 1 shows the feed stock properties, in which $M_{col,0}$ is the amount of feed stock and $x_{col,0}$ is the composition of the feed stock, given by the mole fraction of ethanol. The desired product quality is given by $x_{n+1,sp}^0$, which is measured using a partial least squares (PLS) estimator. To be able to validate the model, three runs are designated as identification runs (ID), the other two are designated as validation runs (VAL).

3. Hybrid modeling

The objective is to develop a hybrid model that can simulate a batch run, including the final two stages of the start-up. Such a model can be used for simulation studies or the optimization of operating conditions, such as the determination of the optimal batch time. However, the main purpose of this work is to investigate the influence of applying additional knowledge in the hybrid modeling approach. Therefore, three different hybrid models will be developed, each incorporating a different level of a priori knowledge.

The measurements limit the level of detail of the hybrid model. No internal data is available, only input–output measurements. In addition, the measurements that are available are obtained from the controlled process. This means that the hybrid models are only valid under similar conditions. The five batch runs describe the column behavior for constant quality control. This means that the process will be simulated using the hybrid models which describe the overall column behavior under this control strategy.

For the development of the hybrid models, a structured modeling approach will be used (Van Lith et al., 2002). This approach consists of three phases. In the first phase, the model objective and model quality requirements are formulated. In the second phase, the hybrid model is designed. This is accomplished by distinguishing the characteristic phenomena that take place and modeling them independently. The model is evaluated in a third phase. This way, the modeling problem is divided into smaller subproblems. If no suitable first principles or empirical representation can

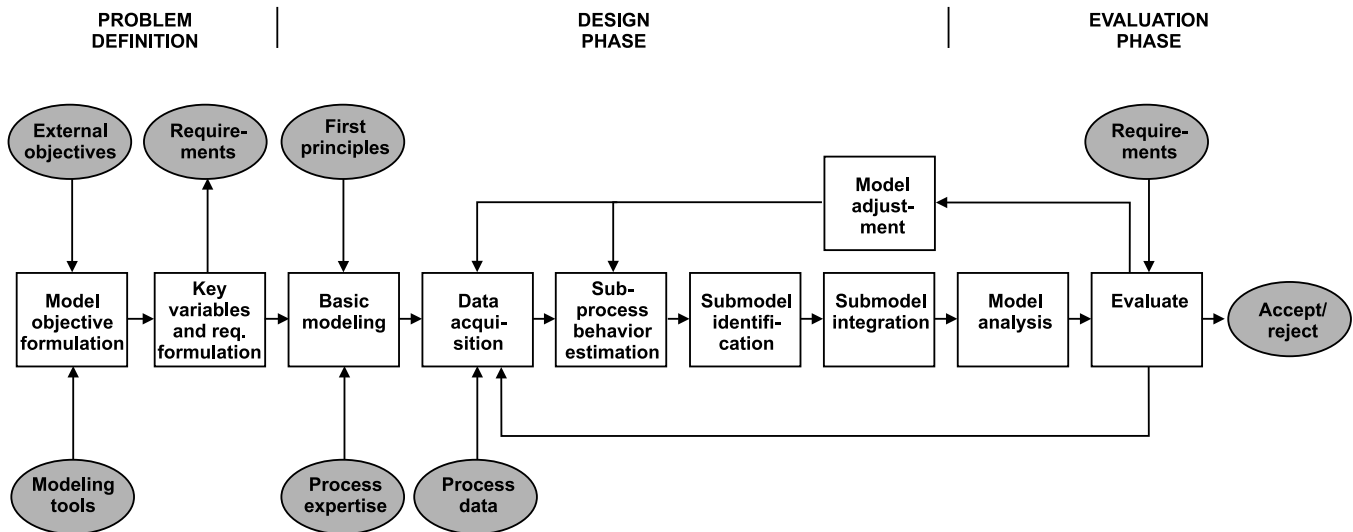


Fig. 2. Hybrid modeling approach.

be derived, fuzzy logic is used. The different submodels are identified and integrated to form the hybrid model. The modeling approach is shown in Fig. 2.

In hybrid modeling as presented in this paper, Takagi–Sugeno–Kang (TSK) type fuzzy models are used (Takagi & Sugeno, 1985). In TSK models, the antecedent part is similar to other fuzzy models, while the consequent part of each rule consists of a linear equation. This type of fuzzy models can be interpreted as a collection of local linear submodels and is extremely suitable to describe highly nonlinear relationships based on process data. In addition, the model structure is simple and transparent.

Many good algorithms for the identification of TSK models from data are available, including algorithms with structure optimization. Since fuzzy logic is used to describe phenomena which are poorly understood or difficult to model using first principles, the identification algorithm should require as little a priori structure information as possible. This can be accomplished by using unsupervised learning algorithms, of which fuzzy clustering is a popular form.

The basic idea behind clustering is to divide a set of objects into self-similar groups or clusters. This similarity is often defined as a distance norm to a cluster prototype. Clustering methods are usually based on assumptions about the geometry of the clusters. In the case of TSK models, the assumption is made that the data can be represented by linear subspaces. This way, each cluster yields a rule in the fuzzy model.

Gustafson–Kessel (GK) clustering (Gustafson & Kessel, 1978) in combination with structure optimization (Kaymak & Babuska, 1995) has found to be an effective tool for building TSK models (De Bruin & Roffel, 1996). The GK algorithm represents clusters with a cluster center and cluster covariance matrix and

uses the covariance matrix during the calculation of the distance norm. The advantage is that the clusters can have different shapes, which provides more flexibility to describe complex problems. In addition, it is insensitive to scaling of the data or initialization (Babuska, 1996).

The structure of the fuzzy model can be optimized by ‘merging’ clusters that show a certain degree of conformity (Kaymak & Babuska, 1995). This is based on two criteria, which are evaluated by using the cluster distances and covariance matrix eigenvectors. The first criterion states that if the clusters are almost parallel, then they should be merged. The second criterion states that if two clusters are sufficiently close, then they should also be merged. These criteria can be consolidated into one parameter: the cluster merging threshold. The result of combining the clustering algorithm and the cluster merging algorithm is that the structure of the fuzzy model can be optimized automatically. It must be noted, however, that whether this optimum meets performance requirements depends on the modeling problem and should be investigated carefully by evaluating different values of the tuning parameters of the algorithm: k_0 , the initial number of clusters and γ , the cluster merging threshold.

The GK clustering algorithm requires input–output data. Depending on the hybrid model structure, this can mean that the values of internal variables, which cannot be measured are needed. In such cases, parameter estimation approaches can be used. In this work, a PI-estimator will be used (Van Lith, Witteveen, Betlem & Roffel, 2001). The PI-estimator is structurally similar to a PI-feedback controller. The PI-estimator is used to “control” a model output in such a way that it matches process measurements by manipulating an unmeasured internal variable. The controller output then serves as an estimate of this unmeasured variable. The PI-estimator

performs similar to Kalman filtering for many processes, but is much easier to set up.

4. Basic hybrid model

4.1. Model structure

To describe the overall dynamics of the column, a simplified model comprised of an overall separation approximation, combined with first order dynamics for the exhaustion, has been derived:

$$\frac{dM_{col}}{dt} = -L_V(1 - R^*) \quad (1)$$

$$M_{col} \frac{dx_{col}}{dt} = -L_V(1 - R^*)(x_{n+1} - x_{col}) \quad (2)$$

$$x_{n+1} = f(R^*, x_{col}) \quad (3)$$

in which M_{col} (mol) is the mass of the column; L_V (mol/h), the condensed vapor flow rate; L_D (mol/h), the distillate flow rate; x_{col} , the average molar ethanol fraction in the column; x_{n+1} , the molar ethanol fraction of the product and $R^* = (L_V - L_D)/L_V$ is the reflux fraction. M_{col} and x_{col} are introduced to avoid the need for tray-to-tray equations to describe the column. The production M_p can be calculated as follows:

$$M_p = M_{col,0} - M_{col} \quad (4)$$

The heat supply is constant during normal operation. In addition, the influence of the exhaustion on the vapor flow is rather limited. As a result, the vapor flow during normal operation will be nearly constant ($L_{V,ss}$). However, during the second stage of start-up, the vapor flow at the top will be less, as part of the heat supply will still be required for additional warming-up of the column wall and for the composition shift from volatile to less volatile components. The transition from the initial vapor flow to the steady state value develops gradually and can roughly be modeled by a first-order behavior:

$$\frac{dL_V}{dt} = \frac{1}{\tau_V}(L_{V,ss} - L_V) \quad (5)$$

in which τ_V is the first order time constant that characterizes column heating and $L_{V,ss}$ is the steady state vapor flow for the given heat supply. For Eq. (5), an estimate for the initial condition $L_{V,0}$ should be used such that the equation matches the observed behavior. After the vapor flow reaches the condenser (second stage), the behavior of the flow can be approximated by the first order equation. The start-up behavior of the model before the vapor flow reaches the condenser (first stage) is not incorporated and not represented by the measurements. Therefore, the model describes the final two stages of the startup behavior. Fig. 4 shows that at

the time the condenser is filled, the separation made already an enormous progress and comes close to the requirement.

Eq. (3) describes the separation as a function of the reflux fraction and the average column fraction. This relation is difficult to derive. Relations based on a so-called separation factor have been used, but they only approximate the separation for steady state conditions as they are valid for continuous operation (Shinsky, 1984).

Based on the process data, a fuzzy relation that describes the separation can be derived. Since it is derived from the data, it can match the observed behavior without imposing a functional relation a priori, as is the case with empirical separation factor relations. In addition, the influence of the start-up on the product quality can be taken into account by incorporating the vapor flow in the input space of the fuzzy model. This way, a hybrid model is obtained that includes first order exhaustion dynamics, first order startup dynamics and a static fuzzy relation that describes the product quality. The structure of the fuzzy relation is, therefore, expanded to:

$$x_{n+1} = f_{fuzzy}(R^*, x_{col}, L_V) \quad (6)$$

This basic hybrid model, comprising Eqs. (1), (2), (4)–(6) will be denoted with “Model I”.

4.2. Identification

Identification of the hybrid model involves the determination of τ_V , $L_{V,0}$, $L_{V,ss}$ and identification of the fuzzy relationship for the product quality (Eq. (6)). The time constant τ_V and the steady state value $L_{V,ss}$ were determined by fitting Eq. (5) to the measurements of L_V . In addition, the initial condition $L_{V,0}$ was determined to provide a better approximation. Results are shown in Fig. 3. Table 2 shows the values of τ_V , $L_{V,0}$ and $L_{V,ss}$ for the three identification runs. The final values that will be used in the model are the averages of the values for the three runs.

The behavior of the vapor flow can be described as follows. When the column is heated, the vapor flow slowly builds up in the column before reaching the condenser. This means that during the first part of the start-up procedure, no vapor flow is measured. The measurements start when the vapor flow reaches the condenser. At that moment, the temperature in the column is still rising and settles after about 0.5 h. This results in the vapor flow as shown in Fig. 3.

For the identification of the fuzzy submodel, R^* , x_{col} , L_V and x_{n+1} need to be available. The reflux fraction R^* , the vapor flow L_V and the product quality x_{n+1} are measured. The column quality x_{col} can be obtained by solving Eqs. (1) and (2). This is done for each of the three identification runs. The combined runs result in an

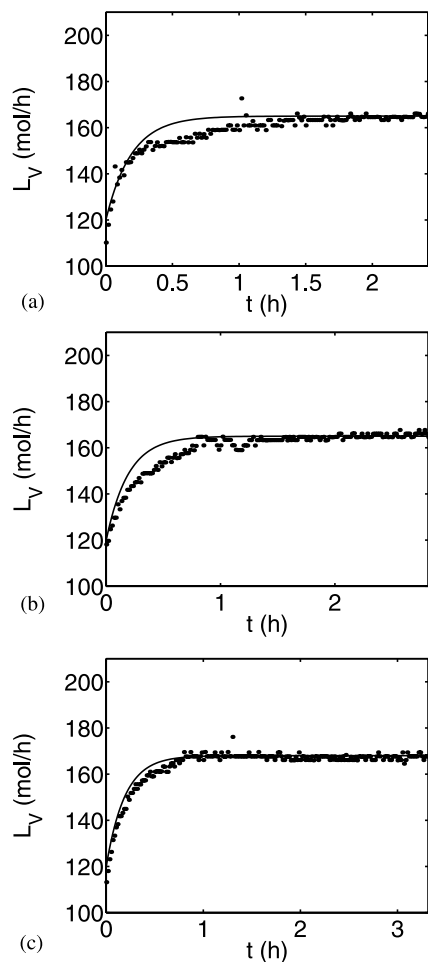


Fig. 3. Model results for L_V , run ID1 (a), ID2 (b) and ID3 (c). Measurements (dots) and model (line).

Table 2
results of parameter estimation start-up dynamics

Run	τ_V (h)	$L_{V,0}$ (mol/h)	$L_{V,ss}$ (mol/h)
ID1	0.2	120	165
ID2	0.2	120	165
ID3	0.2	120	168
Average	0.2	120	166

input–output data set of 512 features. Clustering settings and results are shown in Table 3. The table also gives the root mean squared error with respect to the identification data.

Table 3
Clustering settings and model results for x_{n+1} with: k_0 , the initial number of clusters and γ , the cluster merging threshold

Model	k_0	γ	# Rules	RMSE
I	10	0.7	3	5.3×10^{-4}
II	10	0.6	3	3.6×10^{-4}
III	10	0.6	3	3.7×10^{-3}

The performance of the hybrid model I with respect to the measured model input (R^*) is given in Fig. 4. In this figure, the product quality for the validation batch runs is given. It can be seen that the hybrid model performs acceptably.

During start-up, the quality x_{n+1} is rising. The quality is controlled with a PI controller in combination with a PLS estimator, which estimates the quality from online measurements. This estimator has limited validity and the control loop only works properly if the deviation of the quality from the setpoint is limited. Therefore, the quality controller is switched on if the deviation is less than 0.002 from setpoint. Otherwise, the reflux fraction is set to 1. It takes about 15 min before the controller is switched on.

When the control loop is active, the quality quickly reaches the desired value. There is some “overshoot” present at around $t = 0.5$ h. During warming up of the column, the equilibria on the trays are slightly more in favor of the volatile component than when the column is warmed up. This results in a slightly higher product quality. As the batch run advances, the feed stock becomes exhausted. To maintain the desired product quality, the reflux fraction is increased.

4.3. Simulation

The hybrid model is used to simulate batch runs using the constant quality control strategy. For this purpose, a PI controller is designed which controls the simulated product quality by manipulating the reflux fraction R^* .

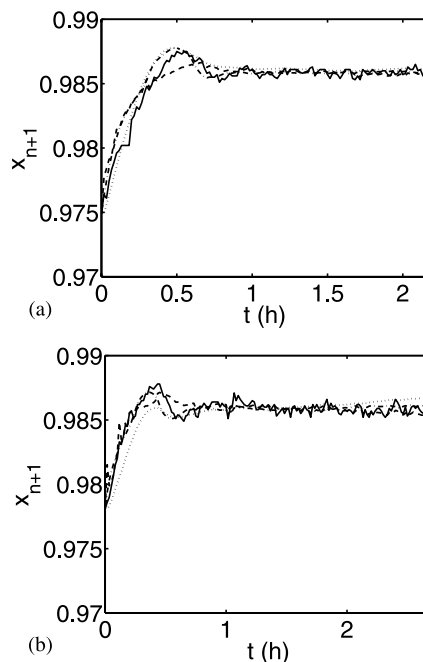


Fig. 4. Hybrid model validation results: measurements (solid line), model I (dashed), model II (dash–dot) and model III (dot), respectively.

Similar to the experimental set up, the controller was switched on if the deviation is less than 0.002 from setpoint. The setpoint was identical to the setpoint for the experimental batch runs and the controller was tuned manually, using trial and error. Settings are given in Table 4. Figs. 5–7 show the results for a simulated batch run with initial conditions taken from ID3. The results for ID1 and ID2 were similar.

The controller was able to achieve good setpoint control quickly (Fig. 5). However, the controller gain is negative for model I. This means that in order to increase product quality, the reflux fraction R^* is decreased. This is in contradiction to what is expected physically and is caused by the fuzzy model. The consequent parameters with respect to R^* (which are a measure for the partial derivatives $\partial x_{n+1}/\partial R^*$) are negative, which locally results in an increase of x_{n+1} if R^* is decreased.

Although the controller achieves constant quality, the reflux fraction R^* is not manipulated in accordance with the experimental results (Fig. 6). On average, the simulated reflux is lower than the measurements, which results in a production, which is higher than the theoretical maximum (when all of the volatile component is recovered, indicated by the horizontal line in Fig. 7).

This behavior is caused by the fact that model I neglects information about the dynamics of the relationship between R^* and x_{n+1} , which is characterized by the dominant time constant. Although the model performs acceptably if measurements of the manipulated variable R^* are supplied, it performs unacceptable during simulation. To improve performance, additional information about the dynamics is required.

5. Basic model augmented with black box dynamics

5.1. Model structure

Information about the dynamics between the relationship of x_{n+1} and R^* is contained to some extent in the measurements, specifically during start-up. This information can be used to construct a dynamic model for the top quality. A first order AutoRegressive with eXogenous input (ARX) approximation will be used. Eq. (6) is replaced by the following equation:

Table 4
PI-controller settings

Model	K	τ_I
I	-12	0.01
II	100	0.10
III	150	0.10

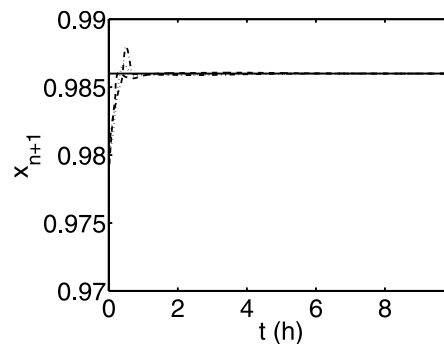


Fig. 5. Quality control results: setpoint (solid line), model I (dashed), model II (dash-dot) and model III (dot), respectively.

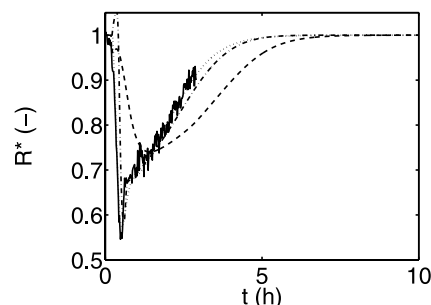


Fig. 6. Reflux fraction R^* : measurements (solid line), model I (dashed), model II (dash-dot) and model III (dot), respectively.

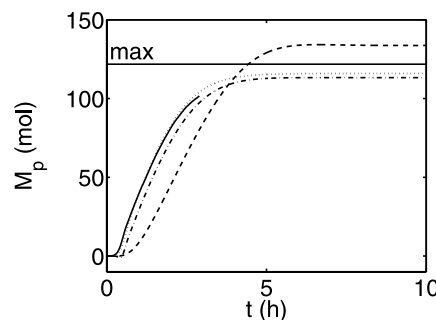


Fig. 7. Production curve: measurements (solid line), model I (dashed), model II (dash-dot) and model III (dot), respectively.

$$x_{n+1,k+1}^0 = f_{fuzzy}(x_{n+1,k}^0, R_k^*, x_{col,k}, L_{V,k}) \quad (7)$$

in which the subscript k denotes the time step. The resulting hybrid model will be denoted with “Model II”.

5.2. Identification

Identification of model II only involves the identification of the fuzzy submodel (Eq. (7)). The other parameters are identical to model I. The fuzzy submodel is identified using fuzzy clustering. Settings are given in Table 3. The model performs well with respect to the measured input R^* of the validation runs (Fig. 4). The “overshoot” around $t = 0.5$ h is described more accurately than with model I, especially for VAL1.

5.3. Simulation

In comparison to model I, model II performs considerably better during simulation. The controller gain K is positive, as would be expected, and quality control is good (Fig. 5). The manipulated variable R^* follows the measurements much more closely (Fig. 6), which indicates that the closed loop dynamics of the simulation approximate the actual experimental setup. However, when the controller is switched on, the reflux fraction is increased and becomes larger than 1, before it is decreased. This was found to be independent of controller tuning and is caused by the fuzzy model. The result is that there is a slight inverse response in the production curve; the production first becomes negative before it increases, which is not possible in practice. The net effect is that the simulated production lags behind the measurements (Fig. 7).

Dynamic information in the measurements of x_{n+1} is only available during the first half hour of a batch run, which represents 20% of the measurements. The simulation results indicate that incorporating dynamics in the relationship between R^* and x_{n+1} improves the simulation, but that the measurements do not provide sufficient information to identify the model parameters accurately.

6. Basic model augmented with dominant time constant

6.1. Model structure

The black box part of the hybrid model is completely data driven. Since the data does not contain sufficient information to identify a dynamic relationship, the dynamic part of this relationship should be obtained in some other way. The dynamic part is represented by the dominant time constant. The dominant time constant can be incorporated by combining a first order dynamic “filter” with a static fuzzy model. The fuzzy model acts as the forcing function of the filter, while the dynamic characteristics are given by the dominant time constant. Eq. (7) is replaced by:

$$\frac{dx_{n+1}}{dt} = \frac{1}{\tau_x} (x_{n+1}^* - x_{n+1}) \quad (8)$$

in which τ_x is the dominant time constant and x_{n+1}^* is the forcing function, given by:

$$x_{n+1}^* = f_{fuzzy}(R^*, x_{col}, L_V) \quad (9)$$

The result is a dynamic relationship for the product quality in which the dynamic characteristics are obtained from prior knowledge and the static characteristics are obtained from measurements. This hybrid model will be denoted with “Model III”.

6.2. Identification

In model III, all parameters are known, except the forcing function (Eq. (9)). Again, the fuzzy model will be identified using fuzzy clustering, for which input–output data is required. The inputs are available, the output is not. Therefore, the output x_{n+1}^* is estimated using Eq. (8) and a PI-estimator. The parameters of the estimator were determined manually. For each of the identification runs, different settings were obtained (Table 5).

Results of the estimates of x_{n+1}^* for ID3 are given in Fig. 8; the other results are similar. The corresponding estimates of x_{n+1} are also given. The estimates are acceptable, although the noise level is higher than in the measurements. This is the result of the filtering effect which Eq. (8) has.

Cluster algorithm settings are given in Table 3. The resulting model performs comparable to model II with respect to the measured input. The product quality lags behind the measurements during the first part of VAL2, while the quality increases somewhat near the end. The lag is caused by the estimation error in x_{n+1}^* , while the increase is the result of the noise in the estimates (as can be seen from the comparison of the RMSE of model I and III, which have similar structure, Table 3), which introduces some bias to the fuzzy model. Since this is an open loop simulation, no feedback is provided to correct the offset. The validation shows the influence of these effects in comparison with model I and II, although the fit to the identification data is acceptable.

6.3. Simulation

Figs. 5–7 show that model III performs better than model I and II. Quality control is good and the simulation matches the measurements of R^* closely. The simulated production curve approximates the measured production well. Switching time is also in accordance with the experimental results. Although the major improvement in model performance was the result of incorporating dynamics in the relationship for x_{n+1} , the results show that the controlled process does not provide sufficient information to derive the dynamic characteristics from the measurements.

Table 5
PI-estimator settings model III

Run	K_{est}	$\tau_{I,est}$
ID1	5	0.04
ID2	5	0.07
ID3	4	0.10

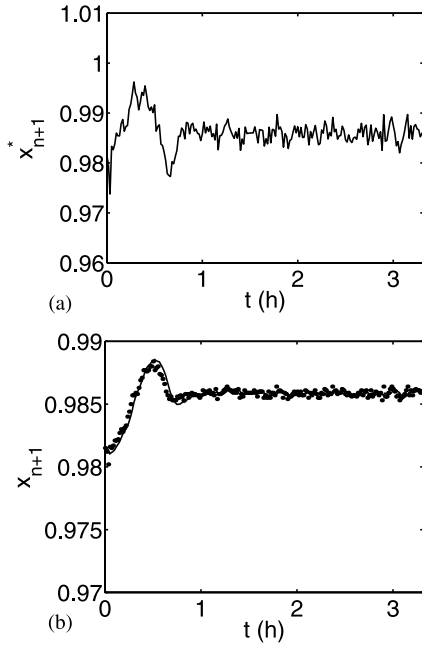


Fig. 8. Estimation results x_{n+1}^* : measurements (dots) and estimates (solid line), respectively.

7. Conclusions

A hybrid fuzzy-first principles model for an experimental batch distillation column has been developed. This model combines general prior knowledge in the form of a dynamic model structure for a batch column operating under constant quality control with specific information about the behavior of the column under study, which is derived from experimental process data. The final derived dynamic framework includes the behavior for bottom exhaustion, column warming-up, and the first-order dynamics of the top-composition, that applies for a column under constant quality or constant temperature operation. This approach results in a relatively simple model, which has the ability to describe the production as a function of the batch time, including part of the start-up, without the need to describe internal column dynamics. This reduces the modeling effort which is required.

The comparison of the different model structures shows that with respect to product quality, the measurements of the controlled process only provide sufficient information to derive static characteristics. Information about the dynamic behavior is incorporated in the form of prior knowledge. By separating the dynamic and static properties during the design of the data driven part of the hybrid model, the information, which the measurements represent is incorporated more effectively.

The model can be improved by taking into account the part of a batch run before the vapor flow reaches the condenser. This requires additional experiments, which allow for data driven development of a model that complements the hybrid model. Based on physical considerations, a model structure can be derived which correlates properties like the amount and composition of the feed stock and energy input to the development of the vapor flow. Fuzzy logic can be used to derive the description from the observations, without the need for rigorous process modeling.

Appendix A: Fuzzy models

The fuzzy MISO models of the form:

$$y = f_{fuzzy}(x_1, x_2, \dots, x_n) \tag{10}$$

with n inputs and m rules are represented by the following set of equations:

$$\mu_{j,i} = \frac{1}{1 + \exp(-a_{k,1}(x_i - a_{k,2}))} \cdot \frac{1}{1 + \exp(-a_{k,3}(x_i - a_{k,4}))} \tag{11}$$

in which $\mu_{j,i}$ is the membership value for input i in rule j and a is the membership function parameter matrix and $k = (i-1)m + j$,

$$\beta_j = \prod_{i=1}^n \mu_{j,i} \tag{12}$$

in which β_j is the degree of fire of rule j ,

$$y_j = \theta \cdot [x_1, x_2, \dots, x_n, 1]^T \tag{13}$$

in which y_j is the output of rule j and θ is the parameter matrix of the consequent part, and

$$y = \sum_{j=1}^m \frac{\beta_j y_j}{\sum_{j=1}^m \beta_j} \tag{14}$$

The parameters of the fuzzy models are given below. Model I:

$$a = \begin{bmatrix} 1.00 & -1000.00 & -41.58 & 0.92 \\ 32.49 & 0.92 & -1.00 & 1000.00 \\ 1.00 & -1000.00 & -1.00 & 1000.00 \\ 38.10 & 0.33 & -41.30 & 0.78 \\ 104.00 & 0.36 & -1.00 & 1000.00 \\ 1.00 & -1000.00 & -45.82 & 0.57 \\ 0.24 & 145.01 & -0.65 & 163.49 \\ 1.00 & -1000.00 & -0.40 & 158.00 \\ 0.20 & 150.00 & -1.00 & 1000.00 \end{bmatrix} \tag{15}$$

$$\theta = \begin{bmatrix} -0.0034 & 0.0023 & -0.0000 & 0.9914 \\ -0.0315 & 0.0083 & 0.0002 & 0.9824 \\ -0.0056 & -0.0022 & -0.0000 & 0.9925 \end{bmatrix} \tag{16}$$

Model II:

$$a = \begin{bmatrix} 38.98 & 0.92 & -1.00 & 1000.00 \\ 12.20 & 0.46 & -33.60 & 0.99 \\ 10.80 & 0.47 & -65.30 & 0.99 \\ 106.00 & 0.36 & -2260.00 & 0.74 \\ 45.80 & 0.33 & -1.00 & 1000.00 \\ 1.00 & -1000.00 & -108.00 & 0.58 \\ 1.00 & -1000.00 & -0.36 & 155.37 \\ 0.54 & 147.00 & -1.27 & 165.00 \\ 0.31 & 153.00 & -1.00 & 1000.00 \\ 1.00 & -1000.00 & -1495.92 & 0.99 \\ 1440.00 & 0.98 & -1.00 & 1000.00 \\ 4490.00 & 0.98 & -8460.00 & 0.99 \end{bmatrix} \quad (17)$$

$$\theta = \begin{bmatrix} -0.0023 & -0.0005 & 0.0000 & 0.8589 & 0.1410 \\ 0.0019 & 0.0009 & -0.0000 & 0.9537 & 0.0441 \\ 0.0023 & 0.0015 & -0.0000 & 0.4994 & 0.4926 \end{bmatrix} \quad (18)$$

Model III:

$$a = \begin{bmatrix} 8.61 & 0.20 & -1.00 & 1000.00 \\ 35.20 & 0.87 & -1.00 & 1000.00 \\ 26.00 & 0.67 & -1.00 & 1000.00 \\ 32.42 & 0.32 & -1.00 & 1000.00 \\ 96.40 & 0.36 & -1.00 & 1000.00 \\ 1.00 & -1000.00 & -14.80 & 0.52 \\ 0.42 & 144.00 & -0.61 & 165.00 \\ 1.00 & -1000.00 & -0.50 & 159.13 \\ 0.67 & 155.63 & -1.00 & 1000.00 \end{bmatrix} \quad (19)$$

$$\theta = \begin{bmatrix} 0.0250 & 0.0182 & -0.0001 & 0.9767 \\ 0.0582 & -0.0477 & 0.0003 & 0.9151 \\ 0.0194 & 0.0147 & 0.0000 & 0.9613 \end{bmatrix} \quad (20)$$

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