NONLINEAR MODEL PREDICTIVE CONTROL OF MULTICOMPONENT DISTILLATION COLUMNS USING WAVE MODELS

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Abstract: A novel control concept for multicomponent distillation columns is presented. The concept is based on nonlinear wave-propagation phenomena that occur in counter-current separation processes. On this basis a reduced order model has been developed in previous work that not only considers profile positions but also the profile shape itself. The reduced model gives direct access to key parameters of the plant, such as the separation front positions. Furthermore, it allows real-time computations for multicomponent distillation columns. Such a model is used for both, the nonlinear model predictive control (NMPC) and the observer design. The observer uses temperature measurements and gives estimated temperature and concentration profile positions as well as compositions in the product streams. The robustness of the observer is shown intuitively and in simulation studies. The control of multicomponent distillation is formulated within the NMPC framework by penalising the deviation of the front positions from their reference points and ensuring the product specifications by means of constraints. By directly taking account of product specifications the presented control concept differs from inferential control schemes known from literature. Due to the fact that the concept is based on simple temperature measurements an industrial application seems easily possible.

Keywords: multicomponent distillation, wave phenomena, nonlinear model predictive control, nonlinear observer

1. INTRODUCTION

In the past a vast number of studies has been done in the area of distillation column control. A review of the work produced in this field until early 90s is given by Skogestad (1997). Most of the approaches consider linear control methods. Although there exist a number of studies on nonlinear control of distillation columns, e.g. (Groebel *et al.*, 1995) they mainly concentrate on high purity binary distillation; a study together with a review on this field is presented in (Balasubramhanya and Doyle III, 1997).

In previous studies tray temperatures are frequently used as controlled variables instead of product compositions (Luyben, 1973; Yu and Luyben, 1984), since temperatures are easily measured online. For high purity binary distillation, the controlled temperatures are easily selected. In general, sensors are located at points where the temperature profile has a sharp transition and this corresponds to some distance away from the column ends. However such inferential control relies on the correlation between the temperature on the measurement trays and the product composition. This correlation becomes poor for multicomponent systems and consequently controlling temperatures alone may result in a considerable violation of the product specifications (Moore, 1992). These difficulties may be overcome by composition estimators derived on the basis of temperature measurements, as proposed by e.g. (Lang and Gilles, 1990; Mejdell and Skogestad, 1991*b*; Mejdell and Skogestad, 1991*a*; Quintero-Marmol *et al.*, 1991; Baratti *et al.*, 1998; Dodds *et al.*, 2001).

In the last decade a new low order modelling approach based on nonlinear wave propagation theory was developed for counter-current separation processes (Marquardt, 1990) taking into account proper profile shapes (Kienle, 2000). This type of wave models offers a more precise insight to the dynamic mechanisms of distillation processes. Additionally they explicitly take into account the separation fronts that determine the quality of the separation.

In (Shin *et al.*, 2000) a nonlinear profile observer together with a profile position control for binary distillation columns is presented. That work makes direct use of the fact that in binary distillation the composition follows from the temperature, which is not possible for multicomponent systems. In contrast, this contribution aims at directly controlling the product composition by adjusting the front position. The capabilities of wave position observers was shown recently in (Roffel *et al.*, 2002) for binary distillation.

Recent developments in the area of nonlinear model predictive control (NMPC) (Allgöwer *et al.*, 1999) provide an efficient control technique that is able to deal with the multi-variable nature of distillation processes and the process operating constraints. Furthermore, it is directly possible to utilise the nonlinear process model.

In this contribution, the advantages of the wave model together with the benefits of NMPC are used to control separation front positions such that the product specifications are met. At the same time further operation limits are respected. Together with an observer that is also based on the wave model, this contribution presents a consistently designed control system that is directly applicable to multicomponent distillation columns.

2. NEW CONCEPT FOR DISTILLATION CONTROL

Most common distillation column models are based on modelling each tray separately. In contrast, the wave model is based on integral balances and regards the concentration profiles by the use of suitable wave functions.

In previous studies it was realized that controlling temperatures on individual trays may have problems in the precences of disturbances in the feed composition. I.e. an adjustment of the setpoints may be come necessary even for binary distillations in order to operate in specification.

Due to these problems wave propagation based concepts have been successfully applied to the control of binary distillation columns (Han and Park, 1993; Balasubramhanya and Doyle III, 1997). An extensions of those concepts to multicomponent distillation columns is not trivial and hence such applications are still missing.

Using the wave model introduced in (Kienle, 2000), the concept can be expanded to multicomponent distillation. In this case there are $N_C - 1$ traveling wave fronts, where N_C stands for the number of components. From among $N_C - 1$ fronts the key separation front has to be selected. The position of this front is used as controlled variable afterwards. The selection can be made by analysing the concentration profiles obtained at the desired operating conditions. The key front is the front which performs the main separation with respect to the product specifications, e.g. in Fig. 2 the fronts s^1_{top} and s^2_{bot} near tray 11 and 40 are selected. The key front is typically a balanced front, i.e. it is a front with zero propagation velocity standing in the middle of a column section.

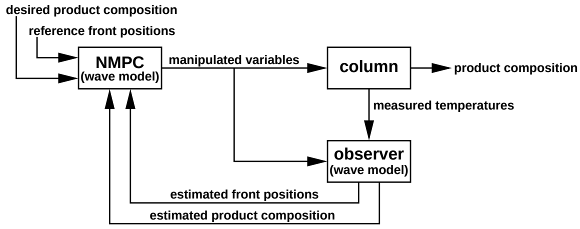

Fig. 1. Control setup

All other fronts are either pushed to the top or bottom of the column section and not able to pass the balanced front. The control aim is to balance the key front in the presence of disturbances and load changes.

2.1 *Control scheme*

Nonlinear model predictive control (NMPC) is chosen as control strategy since it is able to handle constraints on the states. Hence, in contrast to inferential control, the desired product specifications are respected at any time by including them as constraints.

The NMPC technique used in this contribution is based on the following main components: a nonlinear process model, measurements, a state estimator and an optimisation algorithm. As the wave fronts are not measurable, a suitable observer is designed to reconstruct the whole system state by measuring one temperature per column section. In this study, the same nonlinear wave propagation model is employed within both the NMPC and the observer. This makes it less time consuming to set up the complete control environment and only one parameter set has to be identified. The resulting control setup is shown in Fig. 1.

The feasibility of NMPC in real-time by the use of special high performance optimization algorithm is shown in (Diehl *et al.*, 2001*b*; Diehl *et al.*, 2003) for the control of a binary distillation column. Compared to the equilibrium stage model used in (Diehl *et al.*, 2001*b*), which has 42 differential states, a wave model based on similar assumptions only needs 7 differential states. The benefits of such an immense order reduction, are twofold. First it is possible to solve NMPC problems with limited computational power in real-time. Second the NMPC approach can be further exploited by the use of highly sophisticated, more time consuming, optimization strategies.

2.2 *The wave model*

In this section, the used wave model will be sketched, for details the reader is referred to (Kienle, 2000). The column is divided into sections by in- or outflows like feed or side streams. Each of these sections, e.g. the rectifying or the stripping part, is described by a wave model. Wave models are derived from the constant pattern wave phenomena appearing in distillation processes. The main equation is the integral component material balance

$$\frac{dh_i}{dt} = \dot{n}_{i,\mathrm{in}} - \dot{n}_{i,\mathrm{out}} \qquad i = 1 \dots N_C - 1 \qquad (1)$$

over one column section. The integral amount h_i of the component i is calculated with the relation

$$h_i = \sum_{k=1}^{N_S} n_k x_{i,k} \qquad i = 1 \dots N_C - 1 \tag{2}$$

where n is the molar liquid holdup and x_i the mole fraction at each of the N_S trays. The vapour holdup is neglected. Both n_k and $x_{i,k}$ depend on the wave position and are calculated from the wave function. The slope of this wave mainly depends on the wave asymptotes and a mass transfer coefficient. Furthermore, constant relative volatilities and constant molar holdups are assumed.

The other parts of the column like feed tray, condenser and reboiler are described by standard equilibrium models.

3. OBSERVER DESIGN

As pointed out one of the key components of the proposed operating concept for multicomponent distillation columns is the observer. Therefore the main idea is explained in the following and the robustness of the approach is shown intuitively. All ideas will be shown for the case of a ternary distillation, but they can be transfered to distillations with any number of components.

3.1 *Main Idea*

The observer is built up of a plant model that acts as a simulator part and is augmented by an error injection. The error injection is designed by insight into the process dynamics (Lang and Gilles, 1990).

The main idea for the observer design is that the error injection has to try to match the estimated fronts with those of the plant. The following rules for the error injection can be figured out by analyzing the temperature and composition

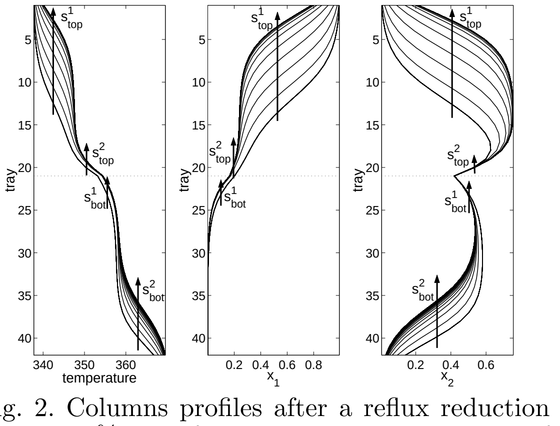

Fig. 2. Columns profiles after a reflux reduction by 25%. The fronts move in the direction of the arrows. The dotted line marks the feed location.

profiles shown in Fig. 2.

The key separating front in the top section, labeled s^1_{top} in Fig. 2, is located near tray 11 at the desired operating point. If the estimated temperature at this tray is too high the front has to be moved down, away from the condenser. This can be achieved by increasing the mole fraction of component 1 and decreasing that of component 2 via error injection.

The same analysis can be applied to the key separating front s^2_{bot} in the bottom section. However, component 1 does not contribute to the movement of the front. Consequently there is no sense in changing the mole fraction of component 1.

This observer design will work in a very robust way since no assumptions regarding the model structure as well as the precise parameter values have been made so far. This idea has been already successfully applied to a reactive distillation column in (Grüner *et al.*, 2001).

In the following the placement of the temperature measurements and subsequently the application of the proposed error injection to the wave model which is used as simulator will be shown.

3.2 *Sensor Placement*

Usually finding the right locations for the sensors is a difficult and important task in the observer design for spatially distributed systems. Wrong sensor placement may even make the process unobservable.

However, for distillation columns nonlinear wave propagation theory provides the necessary information. From the theory it follows, that there can be at most one balanced wave, i.e. a wave with zero propagation velocity in each column section. All other waves are either pushed against the top or the bottom boundary of the column section. Even the smallest changes in the flow rates or the feed composition will make this balanced wave move up or down in the column section. Consequently, this wave is the most sensitive to no matter how small a disturbance to the process is. Thus a temperature measurement in the middle of that front at its nominal location will detect all these movements and is the perfect location for a sensor. In addition to these considerations it should be noted that the control aim is to keep this front at its nominal location. Hence, in stable closed loop operation the wave will never be too far away from the sensor.

3.3 *Error Injection*

As pointed out the idea of the error injection is to move fronts up and down in the column. This can be achieved by injecting the estimation error into the integral component material balances (1) of the wave model. The resulting equation for one section, i.e. either stripping or rectifying section is as follows:

$$\frac{d\hat{\mathbf{h}}}{dt} = \underbrace{\dot{\mathbf{n}}_{\mathrm{in}} - \dot{\mathbf{n}}_{\mathrm{out}}}_{\text{simulator}} + \underbrace{\boldsymbol{\alpha}\left(T_m - \hat{T}_m\right)}_{\text{error injection}}, \tag{3}$$

where T_m is the measured temperature and $\boldsymbol{\alpha}$ the $N_C - 1$-dimensional vector of correction coefficients. The sign of the components of $\boldsymbol{\alpha}$ in the integral material balances is chosen according to the reasoning in Section 3.1. Elements corresponding to compositions that do not contribute to a front movement may be set to zero. In order to reduce the number of tuning parameters, the absolute value of the elements of $\boldsymbol{\alpha}$ is assumed to be equal, resulting in one tuning parameter per column section.

The final magnitude of $\boldsymbol{\alpha}$ can only be determined in closed loop simulation studies. For the following observer performance analysis the $\boldsymbol{\alpha}$ were chosen to be $\boldsymbol{\alpha}_{\text{rect}} = [20, 20]^T$ and $\boldsymbol{\alpha}_{\text{strip}} = [0, -20]^T$.

It is pointed out, that the proposed observer not only gives estimates for the front positions, but also for the complete temperature and composition profiles. I.e., in contrast to e.g. (Shin *et al.*, 2000), it also estimates the product compositions. In addition, the proposed observer is applicable to multicomponent distillation.

3.4 *Observer Performance*

In order to investigate the performance of the proposed observer in the presence of unmeasured disturbances, simulation studies were carried out by using a much more detailed model, representing the plant. This model is a tray to tray constant molar overflow model using saturation pressures to describe the vapour-liquid equilibrium.

Very difficult disturbances to distillation columns are changes of the feed composition as shown in Fig. 3. But even for such a critical disturbance the observer shows good performance.

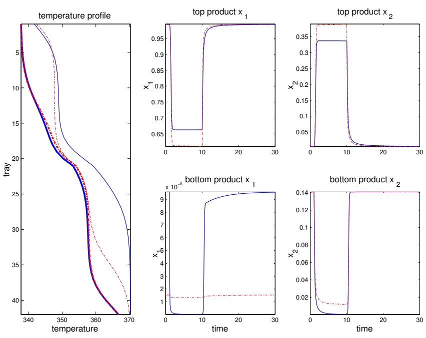

Fig. 3. Response of the observer to a step change of the feed composition at t=1.0 by 10% and back to the nominal value at t=10.0. (Initial profiles in bold, thin profile at t=10.0, solid lines process, dashed-dotted lines observer)

Taking into account that besides other differences the vapour-liquid-equilibrium of the observer model is different from that of the plant model the observer gives good quantitative estimates for the product compositions, especially at the nominal operating point where the estimates are almost indistinguishable from the plant values. Even more important for a good closed loop performance of the observer is its ability to capture the plant dynamics. The time plots of the product compositions shown in Fig. 3 verify that the observer is well able to render the dynamics of the plant.

Besides the simulation study shown in Fig. 3 numerous other simulation studies were done.

These simulation studies show the robustness and good performance of the proposed observer and give full confidence for good closed loop performance.

4. CONTROLER DESIGN

In this study, the nonlinear wave propagation model is employed within the NMPC framework. In the light of the discussion in Section 2 the control aim can be defined as to maintain the wave front positions at their required set points, while at the same time the product specifications have to be fulfilled. This has to be achieved in the presence of disturbances and constraints on the input and output variables.

The process model required for the NMPC framework is a DAE model of index one in the following form :

$$\begin{aligned} \dot{\mathbf{x}}(t) &= f(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t)), \\ \mathbf{0} &= g(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t)), \end{aligned} \tag{4}$$

together with suitable initial conditions, where $x(t)$ and $z(t)$ are the differential and algebraic state vectors, $u(t)$ is the control vector and t is the time.

The NMPC open-loop optimal control problem to solve for a prediction horizon $[0, T_p]$, with horizon length T_p, is given by

$$\min_{\mathbf{u}(\cdot), \mathbf{x}(\cdot)} \int_0^{T_p} \left\{ \|S_i(t) - S_i^{ref}\|_2^2 \right\} dt. \tag{5}$$

The controlled variables are the key front positions, S_i, and desired front positions are denoted by S_i^{ref}. Subscript i corresponds to the column section. The state and control inequality constraints are formulated by

$$c(\mathbf{x}(t), \mathbf{z}(t), \mathbf{u}(t)) \geq 0 \quad \text{for } t \in [0, T_p]. \tag{6}$$

In this particular case

$$c(\mathbf{u}) = \begin{bmatrix} u - u_{min} \\ u_{max} - u \end{bmatrix} \tag{7}$$

define lower and upper bounds for the controls. The important constraints on the top and bottom product compositions, x_T and x_B, are given by

$$\begin{bmatrix} x_T(t) - x_T^{ref} \\ x_B^{ref} - x_B(t) \end{bmatrix} \geq 0 \quad \text{for } t \in [0, T_p]. \tag{8}$$

The constraints on the states, Eq. (8), are treated as soft constraints using slack variables which are added in the objective function as linear penalty terms. Such an approach is particularly useful when output constraints represent the control objectives rather than hard limits in the process.

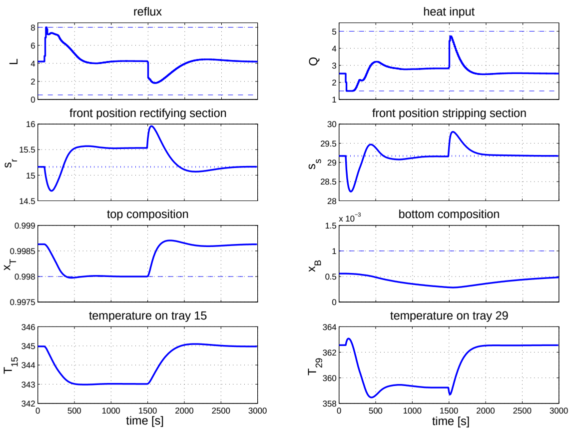

Fig. 4. Closed loop simulation experiment after 50% increase and decreasing to the original value of the light component in the feed. (dashed lines: boundaries, dotted lines: setpoints)

To ensure nominal stability of the closed system a practical approach based on the result given in (Chen and Allgöwer, 1998) was taken. This is done by dividing the prediction horizon into a control horizon $[0, T_c]$ and a prediction interval $[T_c, T_p]$ along which the controls are kept constant at their final values.

In order to show the advantage of the proposed control concept at first a NMPC closed loop simulation study for the binary separation of methanol and 1-propanol is presented in Fig. 4. Controlling the only existing front in the binary problem is equivalent to controlling the key separation front in the ternary case.

The reflux flow-rate, L, and the heat input, Q, into the reboiler (which corresponds to the vapour flow rate out of the reboiler) are considered as manipulated variables (LV configuration).

The scenario considered in the following is a 50 % step increase of the light component in the feed occurring after 100 seconds and a decrease to its original value after 1500 seconds. T_c, is selected as 1200 seconds with 10 control intervals and T_p is 30000 seconds. The product concentration constraints are set to $x_T(t) \geq 0.998$ and $x_B \leq 0.001$. As shown in Fig. 4 the fronts have to be shifted to fulfill the product specification at the top of the column. After the disturbance disappeared the fronts are shifted back to their reference points.

If one chooses the inferential control scheme for the same binary distillation system, the controlled temperatures would be on trays 15 and 29 similar to (Diehl *et al.*, 2003) and as Fig. 4 clearly shows, set-points of the temperature controllers have to be modified to guarantee the product specifications.

The NMPC computations are carried out on a Unix workstation running under Linux (1 Ghz AMD Athlon processor), using an efficient dynamic optimisation algorithm which is based on a direct multiple shooting approach and available

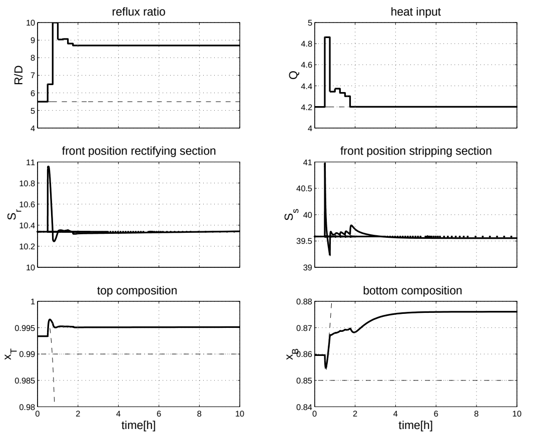

Fig. 5. Open loop simulation experiment after 33% decrease of the light component in the feed. (dash-dotted lines: boundaries, dotted lines: setpoints, dashed lines: uncontrolled)

as the dynamic optimisation software, MUSCOD-II (Diehl *et al.*, 2001*a*).

The application of the control concept to multicomponent systems is demonstrated for the ternary system of methanol/ethanol/1-propanol. The two key fronts to be controlled are s^1_{top} and s^2_{bot} located near tray 11 in the rectifying section and near tray 40 in the stripping section at the nominal operating point respectively. Manipulated variables, the reflux ratio, L/D, and the heat input, Q (L/D,V configuration) are computed in 6 control intervals each of 900 seconds length and T_p is 30000 seconds.

Fig. 5 shows the input and state trajectory obtained as a solution to the NMPC open loop optimal control problem in the face of a disturbance in the feed concentration (33 % step decrease of the light component). The key front positions, S_r and S_s are kept nicely around desired reference values. Meanwhile constraints on the product concentrations, $x_T \geq 0.99$ and $x_B \geq 0.85$, are satisfied. The dynamic optimisation problem for *Case II* was solved within the process simulation environment DIVA(Kröner *et al.*, 1990). A standard Sequential Quadratic Programming (SQP) algorithm from NAG library is used. [1]

5. CONCLUSION

A novel concept for the control of multicomponent distillation columns has been proposed. The main idea of the control concept is based on the observation that the product composition is mainly influenced by the key separating front.

The control achieves the desired product specifications by adjusting the position of the key separation front in each column section, while the product specifications are ensured by constraints in the NMPC. Due to the fact that a direct specification of the product composition is possible,

[1] Current work is on the NMPC closed loop application for the ternary system within MUSCOD-II environment and results are likely to be presented at the conference.

the control concept is a direct control concept in contrast to the many inferential control concepts in the literature. The capability of the concept was shown in two case studies for a binary and a ternary distillation.

The NMPC is provided with the necessary information by an observer. Both, observer and NMPC use the same wave model. The robustness of the observer with respect to parameter errors as well as model-plant mismatches is intuitively shown and validated by simulation studies for a ternary separation.

In the future the control concept will be applied to a ternary separation of e.g. methanol/ethanol/1-propanol in a system of two coupled distillation columns. This will be done first in simulation studies and then at the pilot scale plant at the Institut für Systemdynamik und Regelungstechnik.

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