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Model Predictive Control of a Kaibel Distillation Column

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Abstract: This is a simulation study on controlling a Kaibel distillation column with model predictive control (MPC).
A Kaibel distillation column has several advantages compared with conventional binary column setups. The Kaibel column separates a feed stream into four product streams using only a single column shell. The distillation process is a multivariable process which leads to a multivariable control problem. The objective for optimal operation of the column is chosen to be minimization of the total impurity flow. An offline optimization on a mathematical model leads to temperature setpoints to be used by a controller. An MPC generally obtain less total impurity flow compared to conventional decentralized control when the distillation column is exposed to disturbances. It also counteract process interactions better than decentralized control.

Keywords: Kaibel distillation column, multivariable control system, model based control

1. INTRODUCTION

This paper describes an implementation of a model predictive controller of a Kaibel distillation column (Kaibel, 1987). The presented results are based on a simulation model of the column. A Kaibel distillation column is a thermally coupled distillation column that separates a feed stream into four product streams in a single column shell (see fig. 1). A conventional binary column setup would require three binary columns to separate into four product streams, and hence three reboilers.

A Kaibel distilllation column is an extension of the Petlyuk column (Petlyuk et al., 1965). The Petlyuk column and the dividing wall column (Wright, 1949) have been extensively investigated in literature. Comparison of different control strategies for dividing wall columns are presented in van Diggelen et al. (2010).

The motivation for using a Kaibel distillation column compared to a conventional binary column setup is mainly three reasons:

- Less energy consumption (20 - 40 %)
- Less investment capital required
- Less physical space required in a process plant

One of the main challenges that come with use of the Kaibel column is in the field of control. The energy savings are not achieved if the distillation column does not operate around its optimal operating points. The column is a multivariable process that gives motivation for use of a model
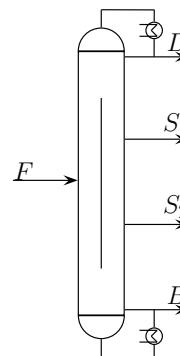

Fig. 1. Kaibel distillation column: Feed stream F, top product stream D, side product streams S_1 and S_2 and bottom product stream B.

predictive controller (MPC). An MPC finds the optimal inputs to the process by use of mathematical optimization based on a mathematical model of the process. An MPC does also naturally take care of constraints in the process, e.g. input limitations.

A pilot plant of the Kaibel column has been built at Department of Chemical Engineering, NTNU. This column uses the alcohols butanol, ethanol, methanol and propanol as feed. The modelled column to be presented is similar to this experimental column. Experimental runs of the pilot

Table 1. Inputs to the column model.

Variable	Explanation	Nominal value	Unit
L	Reflux	2.8492	mol/min
V	Vapor boil-up	3.0000	mol/min
S_1	Sidestream 1	0.2494	mol/min
S_2	Sidestream 2	0.2497	mol/min
R_L	Liquid split	0.2572	-
R_V	Vapor split	0.3770	-
F	Feed stream	1.0000	mol/min
z_D	Mole fraction of D in feed	0.2500	-
z_{S_1}	Mole fraction of S_1 in feed	0.2500	-
z_{S_2}	Mole fraction of S_2 in feed	0.2500	-
q	Liquid fraction of feed	0.9000	-
D	Top product	0.2508	mol/min
B	Bottom product	0.2503	mol/min

plant have verified that the Kaibel column is a process that is difficult to control since the process is nonlinear and have considerable interactions. A picture of the experimental column can be seen in fig. 3. The laboratory column is not implemented directly with a dividing wall, but has instead two branches where each branch represents each side of the wall in a corresponding dividing wall column.

More details and additional simulations for the Kaibel column are found in Kvernland (2009).

2. DISTILLATION MODEL

A stage-by-stage model is used for modelling of the Kaibel column. Wilson's model is used to model the vapor-liquid equilibrium on a column stage. The column is divided into seven column sections, and each of these sections are divided into column stages. The simulated column model has totally 64 stages which is shown in fig. 2. The stages are numbered with the prefractionator sections first. The inputs are defined in Table 1 and are divided into manipulated inputs (u) and inputs that are considered as disturbances (d):

$$u = [L \ S_1 \ S_2 \ R_L \ D \ B]^\top, \qquad (1)$$

$$d = [V \ R_V \ F \ z_D \ z_{S_1} \ z_{S_2} \ q]^\top. \qquad (2)$$

Note the mole fraction notation where the subscript represents the key component in the actual flow, e.g. the amount of key distillate in the feed flow is z_D, and x_D in the top product flow. Also note that the vapor split (R_V) is considered as a disturbance in this work. Initially the vapor split was thought to be a manipulated input, but it has shown to be very difficult to control the vapor flows in practice.

The full distillation model with mass balances, mole fraction balances and temperature differential equations for all 64 stages gives a state space model with almost 350 states. The temperature differential equations comes from a simple update law for the temperature at each stage. The column is built with an open vent, which means that the pressure inside the column will tend to atmospheric pressure P_0. To make sure that the pressure at each stage converges to P_0, the stage temperature is adjusted:

$$\frac{\mathrm{d}T_k}{\mathrm{d}t} = \mu \left(P_0 - P_k(x_{i,k}, T_k) \right), \qquad (3)$$
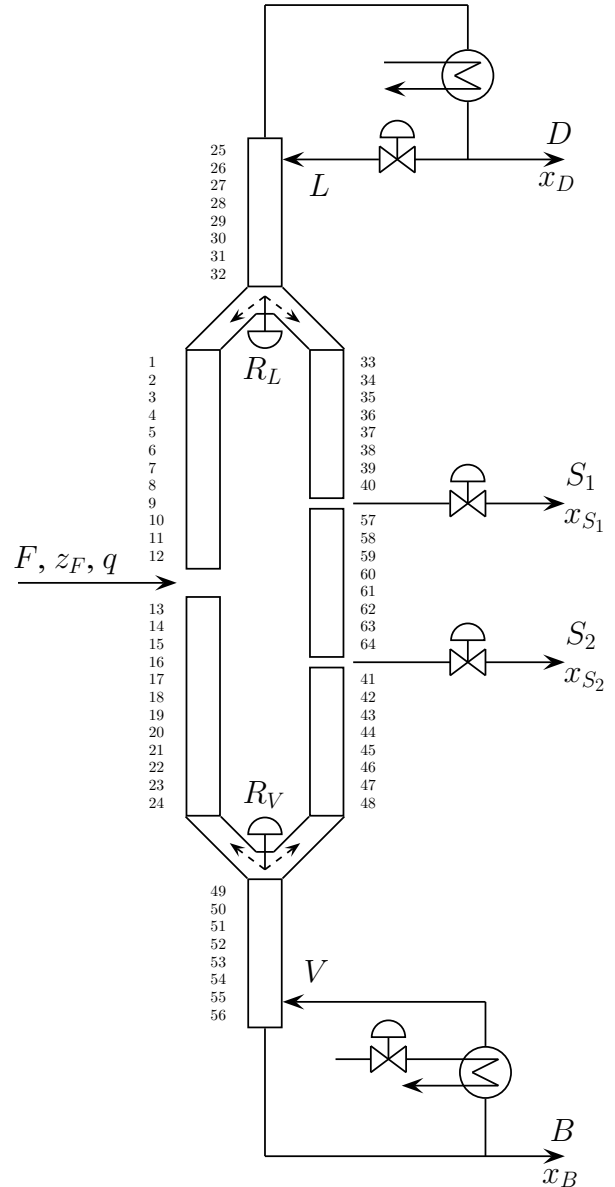

Fig. 2. The modelled column showing the seven sections and the 64 stages. $z_F = [z_D \ z_{S_1} \ z_{S_2}]^\top$. z_B is given by the three others since the total mole fraction adds up to unity.

for all stages k and feed components i. The stage pressure P_k is found by Wilson's model. μ is a positive constant that decides the speed of convergence.

The model is also strongly nonlinear due to the vapor-liquid equilibrium and the mixing terms in the component mass balance at each stage.

The model was further extended to include heat loss and vapor bypassing to describe insufficient mixing at column stages. These model extensions were done to make better fit of simulation data compared to experimental measurements. A model summary is given in app. A.

3. CONTROLLING THE COLUMN

3.1 Performance objective

We consider a case with a given feed rate F and a given vapor boil-up V. Note here that given (maximum) boil-up is usually the optimal mode of operation when energy is cheap. The objective is then to optimize the product distribution. We assume that there are no purity constraints but that we only get paid for main component in each product. With equal prices for the products the objective is then equivalent to minimizing the sum of the impurity flows. The cost function J_{ss} can then be written as (Strandberg, 2008):

$$J_{\text{ss}} = D(1-x_D) + S_1(1-x_{S_1}) + S_2(1-x_{S_2}) + B(1-x_B) \quad (4)$$

The cost J_{ss} was minimized with respect to the inputs given by eq. (1) in addition to the vapor split (R_V), giving optimal input values presented as "nominal values" in table 1. In steady state operation the column model returns the following nominal product purities:

$$x_{\text{nom}} = \begin{bmatrix} x_{D,\text{nom}} \\ x_{S_1,\text{nom}} \\ x_{S_2,\text{nom}} \\ x_{B,\text{nom}} \end{bmatrix} = \begin{bmatrix} 0.9703 \\ 0.9361 \\ 0.9589 \\ 0.9949 \end{bmatrix}. \quad (5)$$

3.2 Level and temperature control

The inputs given by eq. (1) must be manipulated from a controller. The top and bottom product streams (D and B) are chosen to be used for control of the condenser and reboiler levels respectively. These product streams are controlled by PI-controllers with specified level setpoints. The rest of the inputs are used for *temperature control*. Temperature control is an efficient and simple way of controlling the purities indirectly. Temperatures along the column have a good correlation with the product purities inside the column (Skogestad, 2007). Hence, the control structure is divided into level control and composition control (temperature control).

Temperatures at the column stages 17, 30, 49 and 59 are chosen as control variables for the temperature loops, i.e.

$$y = [T_{17}\ T_{30}\ T_{49}\ T_{59}]^\top. \quad (6)$$

This output stage selection is done as a part of earlier work (Strandberg and Skogestad, 2006). Here the minimum singular value method (Halvorsen et al., 2003) was used.

The temperature setpoint values are easily found from the distillation model when the presented optimal inputs in eq. (5) are applied in steady state operation:

$$y_{\text{nom}} = \begin{bmatrix} T_{17,\text{nom}} \\ T_{30,\text{nom}} \\ T_{49,\text{nom}} \\ T_{59,\text{nom}} \end{bmatrix} = \begin{bmatrix} 368.29\,\text{K} \\ 341.97\,\text{K} \\ 379.64\,\text{K} \\ 355.83\,\text{K} \end{bmatrix}. \quad (7)$$

3.3 Decentralized control

A decentralized controller is the simplest way of designing a multivariable controller. Each process output is controlled by a linear controller from a selected input. For the Kaibel column T_{17} was chosen to control the liquid split (R_L), T_{30} controls the reflux (L) and T_{59} and T_{49}

(a) Decentralized control of the Kaibel column. The figure shows the four temperature loops.

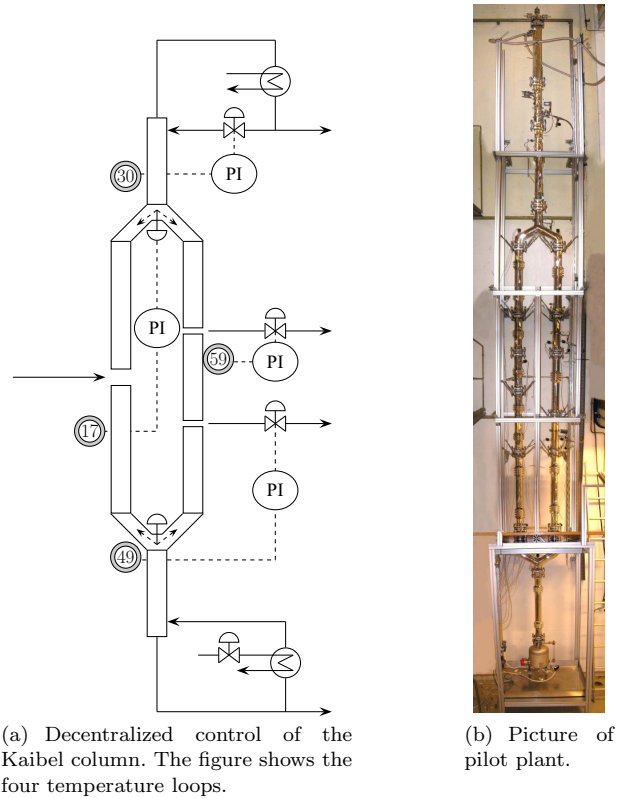(b) Picture of pilot plant.

Fig. 3. Decentralized control structure and pilot plant at NTNU.

controls side stream 1 and 2 respectively (S_1 and S_2). Each temperature measurement is fed into a PI-controller controlling its respective process input, shown in fig. 3(a).

The decentralized PI-controller loops were tuned individually using Simple / Skogestad Internal Tuning Rules (SIMC) (Skogestad, 2003).

3.4 Model predictive control

MPC is an appropriate way to control a multivariable process with considerable interactions such as the Kaibel column.

Two different MPCs have been made; a single layer MPC that controls the real process inputs, and a supervisory MPC controlling the setpoints of a decentralized control layer. The two control structures are shown in fig. 4.

The level controllers are still ordinary PI-controllers, it is the composition control that is handled by the MPC. The objective for the MPC controllers is to minimize the temperature deviations from the pre-computed setpoints.

Using the original performance objective in the MPC, the total impurity flow, would require estimation or measures of the product purities when the column is in operation. This is not considered here.

The internal prediction model used by the MPC to find optimal process inputs is made from the presented distillation model. The prediction model is derived from linearization of the full nonlinear model, and not from step-response experiments. Since the state space model consists of almost
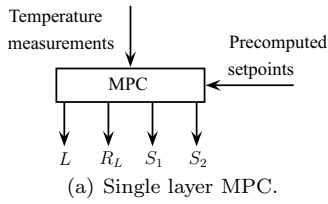
(a) Single layer MPC.
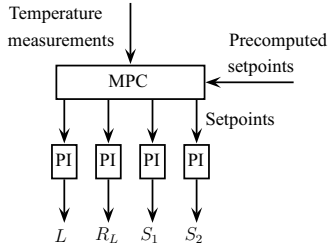
(b) Supervisory MPC.

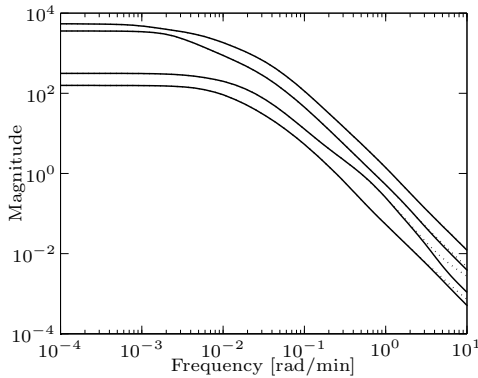Fig. 4. The different MPC control structures.

Fig. 5. Singular values for the linearized model with L, S_1, S_2 and R_L as inputs and the four temperatures as outputs. Original linearized model (solid) and reduced model (dashed).

350 states, it is hard to use this large model inside an MPC optimization problem. The linearized model was therefore reduced down to 20 states. The reduced model of order 20 did not affect the dynamic behaviour for relevant frequencies too much compared to the full linear model. This is verified by plotting the singular values in fig 5 for the two linear models. The singular values for the system gives information about the gains of the process (Skogestad and Postlethwaite, 2005). Plotting the singular values around closed loop frequencies gives a good indication of how good approximation the reduced model is. Linear models of even less order than 20 were tested (10 and 15), but simulations with such orders did not give robust control. However, sufficient robustness was obtained with a model order of 20, which is still considerably less than the full model. The robustness was tested by simulating a set of setpoint changes, disturbance and model parameter errors. The states in the reduced model no longer represent actual physical properties like stage compositions and temperatures.

MPC Toolbox in Matlab was used for implementation of the MPCs. The optimization problem used by the MPC is presented in Bemporad et al. (2009). It uses quadratic expressions and weighs the output reference error $(y -$

$y_{\text{nom}})$ and input changes from one time step to the next (Δu). Hence, the MPC objective function can be written as:

$$J_{\text{dyn}} = \sum_{i=1}^{4} w_i^y \left(y(i) - y_{\text{nom}}(i) \right)^2 + \sum_{j=1}^{4} w_j^{\Delta u} \Delta u(i)^2 \quad (8)$$

Note that this dynamic optimization objective J_{dyn} is unlike the steady state objective (J_{ss}) given in eq. (4).

The weights for the single layer MPC were chosen as:

$$w_{T_{17}}^y = w_{T_{30}}^y = w_{T_{49}}^y = w_{T_{59}}^y = 1 \quad (9)$$

$$w_L^{\Delta u} = w_{S_1}^{\Delta u} = w_{S_2}^{\Delta u} = w_{R_L}^{\Delta u} = 1 \quad (10)$$

The supervisory MPC had similar weights for the output reference error, but less weights on the input changes; $w_L^{\Delta u} = w_{S_1}^{\Delta u} = w_{S_2}^{\Delta u} = w_{R_L}^{\Delta u} = 0.01$.

Improved performance may be obtained by suitable fine tuning of the weights and parameters, but this was not investigated further in this work.

Input constraints were added to the MPC such that unrealistic inputs were avoided. The liquid split (R_L) and the side streams $(S_1$ and $S_2)$ were constrained to a maximum value of 1, the reflux flow to 3.

10 min was chosen as the sampling time of the MPC and a prediction horizon equal to 50 timesteps, i.e. 500 min. The control horizon is equal to the prediction horizon.

4. SIMULATIONS

The simulations were done in Matlab. In the MPC, the states were updated by an observer based on the measurements from "the plant", here realized by the full nonlinear model.

4.1 Disturbance tests and setpoint change

To compare the controller performance different disturbance tests were performed. It is important that the distillation column is able to handle changes in the feed since this flow is determined by other parts of the process plant where this column is in operation. Therefore the controlled column has been tested for changes in the feed flow and feed composition. The vapor split is a degree of freedom with great uncertainty and is therefore included in the disturbance tests.

Interactions in the process and how the controllers counteract these interactions, can be seen in a simulation with a change in one of the temperature setpoints.

4.2 Disturbance responses

Temperature responses are shown in fig. 6. Fig. 7 shows the performance objective value versus time for the corresponding simulations. From the responses in fig. 6 and 7 we see that the MPCs have a generally better performance than the decentralized controller (solid line). The single layer MPC reaches the respective setpoints quite slow but has the least overshoot after a disturbance.

4.3 Change in the setpoint for T_{17}

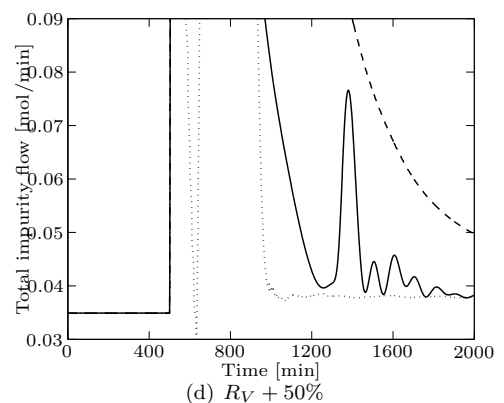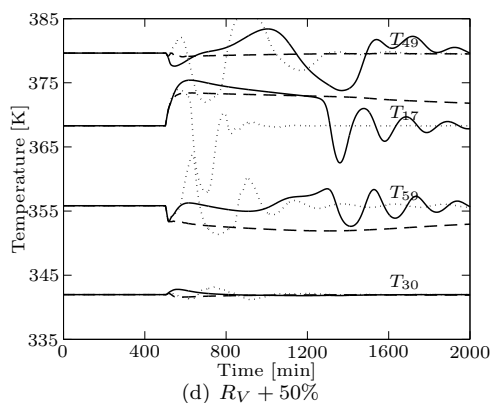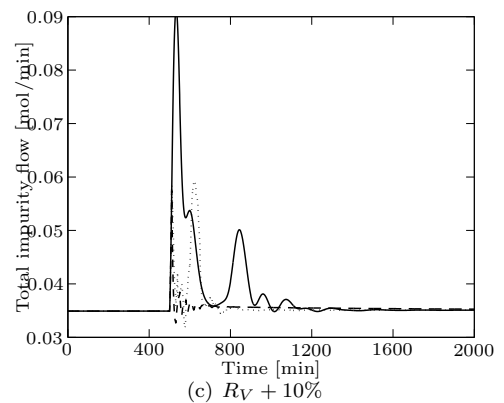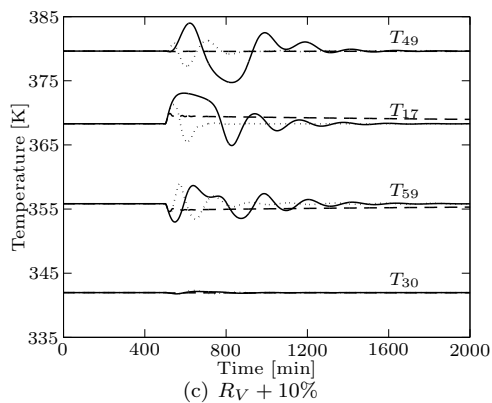Fig. 8 show the controlled temperatures when one of the setpoints is changed.

(a) $F + 10\%$

(b) $z_{S_1} + 20\%$
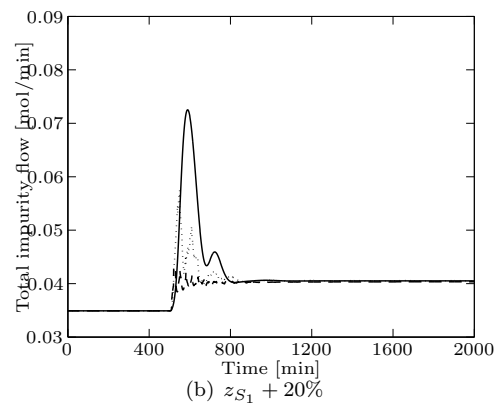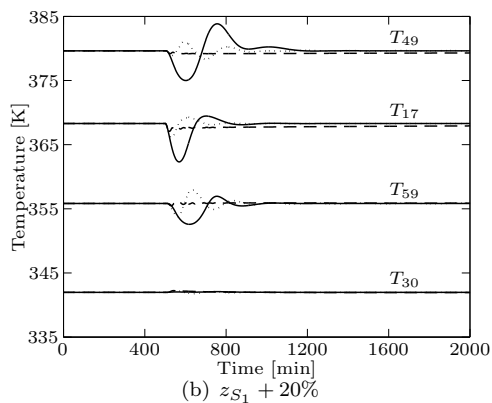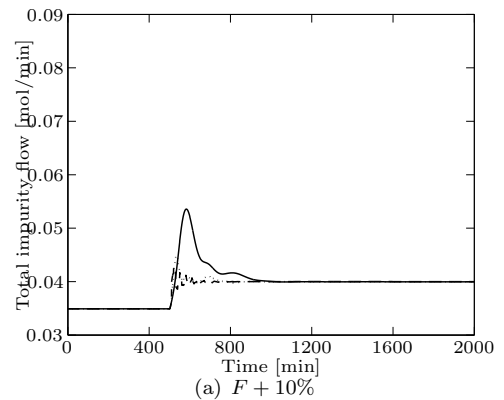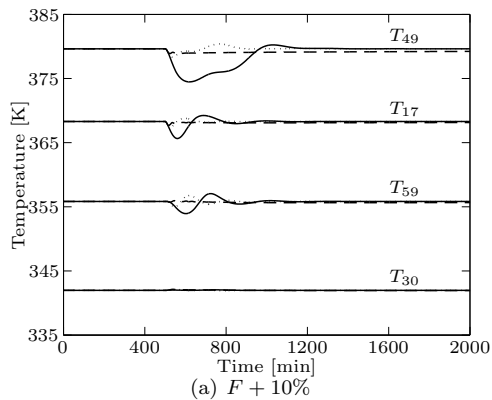
(c) $R_V + 10\%$

(d) $R_V + 50\%$

Fig. 6. Plots showing the controlled temperatures affected by different disturbances. Decentralized PI-control (solid), single layer MPC (dashed), MPC combined with PI-control (dotted). The disturbances occured at time 500 min.

(a) $F + 10\%$

(b) $z_{S_1} + 20\%$

(c) $R_V + 10\%$

(d) $R_V + 50\%$

Fig. 7. Total impurity flow. Decentralized PI-control (solid), single layer MPC (dashed), MPC combined with PI-control (dotted). The disturbances occured at time 500 min.
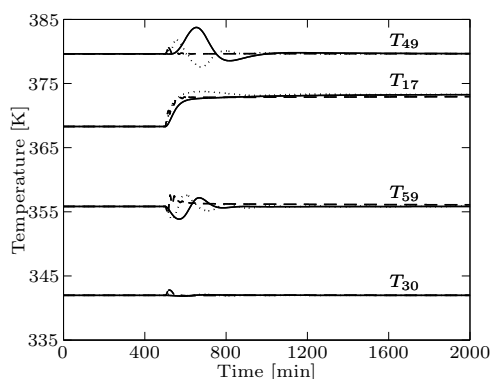
Fig. 8. Setpoint change for T_{17} $(+5\,\mathrm{K})$ at time $500\,\mathrm{min}$. Decentralized PI-control (solid), single layer MPC (dashed), MPC combined with PI-control (dotted).

4.4 Robustness simulations

A large number of simulations were performed in the work of Kvernland (2009) to check the robustness of the different controllers. Simulations with input gain error, time delay and increasing insufficient mixing at column stages (vapor bypassing) were tested. The simple decentralized controller and the supervisory MPC gave best performance.

5. CONCLUSIONS

An MPC is verified to be an appropriate controller for a Kaibel column through simulations. The MPC with a linear reduced order model performed satisfactorily even if the full model is nonlinear with a large number of states.

An MPC generally achieves less impurity flow during disturbances and reduces interactions in the process compared to a decentralized controller. Fig. 8 shows that the MPCs reduce process interactions more compare to a decentralized controller. A supervisory MPC is preferable since it performs better than a single layer MPC during robustness tests.

5.1 Further work

The authors want to see how the MPC works in practice by using it to control the experimental column built at NTNU.

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Appendix A. DISTILLATION MODEL SUMMARY

Table A.1. Distillation model summary.

A single simulation step in the simulation model	
1	Compute liquid and vapor flows for each stage k in the column, i.e. determine: $L_k, \forall k$, where the liquid input of stage 25 is given (see fig. 2) $V_k, \forall k$, where the vapor input of stage 56 is given (see fig. 2)
2	Compute change in mass for each stage k using the differential equation for mass balance: $\frac{dM_k}{dt} = L_{k+1} - L_k + V_{k-1} - V_k$
3	Compute vapor mole fraction for each component i at each stage k: $y_{i,k} = \frac{x_{i,k}\gamma_{i,k}p^0_{i,k}(T_k)}{P_k}$, where the activity coefficient $\gamma_{i,k}$ is found by Wilson's model and the pressure at stage k is: $P_k(x_{i,k}, T_k) = \sum_{i=1}^{N_c} x_{i,k}\gamma_{i,k}p^0_{i,k}(T_k)$ (liquid mole fraction $x_{i,k}$ and temperature T_k used in these equations comes from the previous simulation step)
4	Compute liquid mole fraction for each component i at each stage k: $\frac{dx_{i,k}}{dt} = \frac{1}{M_k}(L_{k+1}(x_{i,k+1} - x_{i,k}) - V_k(y_{i,k} - x_{i,k}) + V_{k-1}(y_{i,k-1} - x_{i,k}))$
5	Update temperature at each stage k: $\frac{dT_k}{dt} = \mu(P_0 - P(x_{i,k}, T_k))$