Control of divided wall columns

Research Project / Forschungspraktikum Ausland

Moritz Gleinser
(Matrikel Nummer/Studet number: 3126710)
July 13, 2013

Betreuer TU München:	PROFESSOR DR.-ING. KAI-OLAF HINRICHSEN Technische Universität München (TUM) Lehrstuhl I für Technische Chemie Lichtenbergstr. 4 D-85747 Garching, Deutschland
Supervisor NTNU	PROFESSOR SIGURD SKOGESTAD Norwegian Univ. of Science and Technology (NTNU) Department of Chemical Engineering Sem Sælands vei 4 N-7491 Trondheim, Norway

Acknowledgment

This work was written during an exchange program at the Norwegian University of Science and Technology in Trondheim. I wish to express special thanks to Professor Sigurd Skogestad for being my supervisor and for this great opportunity. I really had a good time in Norway and especially with his process control group.

Furthermore I would like to thank Deeptanshu Dwivedi, who was writing his PhD thesis about the control of three- and four-product columns. He introduced me to the core program and helped me with many discussions about the simulations.

I would also like to thank Professor Dr.-Ing. Kai-Olaf Hinrichsen for supporting my exchange to Norway and supervising my final report.

Abstract

In this work different control structures for a three-product Petlyuk column are compared. The selection contains two different composition controls, a temperature control and the development to cascade control setups. All of them are tested with large disturbances in the feed rate and feed composition.

The main part is about the implementation of the control structures and the overall rating of their performance and stability. An overview of the strengths and weaknesses of the different layouts is given as well as some general recommendations for the tuning of these complex control structures.

Contents

List of Tables V

List of Figures VII

1 Introduction 1

2 Theory 3
- 2.1 Petlyuk Column 3
- 2.2 Controller Tuning Rules 5
  - 2.2.1 SIMC tuning rules 5
  - 2.2.2 Tuning procedure 6

3 Simulation Models 7
- 3.1 Basics of the MATLAB model and steady state 7
- 3.2 Control Structures 9
  - 3.2.1 Initial Control Structure (Setup 1) 9
  - 3.2.2 Setup 2: Control of side stream purity with boil-up 10
  - 3.2.3 Setup 3: Temperature control 10
  - 3.2.4 Setup 4: Cascade Control 15
  - 3.2.5 Setup 5: Cascade Control with fixed Vapor Split 17
  - 3.2.6 Setup 6: Partial Cascade Control 19

4 Results and Discussion 21
- 4.1 Initial Control Structure (Setup 1) 21
- 4.2 Setup 2: Control of side stream purity with boil-up 21
- 4.3 Setup 3: Temperature control 24
- 4.4 Setup 4: Cascade Control 27
- 4.5 Setup 5: Cascade Control with fixed Vapor Split 27
- 4.6 Setup 6: Partial Cascade Control 29

5 Conclusion 31

Bibliography 33

List of Tables

3.1 Parameters of the model 7
3.2 Steady state values 9
3.3 Nominal Flow rates 9
3.4 Initial controller pairing and tuning parameters 10
3.5 Controller pairing and tuning parameters of Setup 2 11
3.6 Stages and nominal values for the temperature control (Setup 3) 15
3.7 Tuning parameters of the cascade control (Setup 4) 17
3.8 Tuning parameters of the cascade control with fixed vapor split (Setup 5) 18
3.9 Tuning parameters of the partial cascade control with fixed vapor split(Setup 6) 19

5.1 Performance of the different control structures ($--$ error, $-$ constraints not reached, o constraints slowly reached($> 300\,\text{min}$), $+$ constraints reached ($< 300\,\text{min}$), $++$ constraints quickly reached($< 100\,\text{min}$)) 31

List of Figures

1.1 Thermally and mass-coupled setup according to Petlyuk 1

2.1 Direct and indirect sequence to separate a mixture of the three components A, B and C (Condensers and reboilers are not shown) 3
2.2 More advanced structures to separate three components A, B and C . . . 4
2.3 Combination of the prefractionator and the main column into one divided wall column 4
2.4 Step response to a change of the controlled value u(t) 5

3.1 Implementation of the Petlyuk structure 8
3.2 Control structure of setup 1 11
3.3 Control structure of setup 2 12
3.4 Control structure of setup 3 / Temperature Control 13
3.5 Temperature changes in the prefractionator and the main column for changed controller values 14
3.6 The temperature profile does not change for feed rate variations, while changes in the feed composition have an obvious effect on it 15
3.7 Control structure of setup 4 / Cascade Control, with primary loop (index 1) and secondary loop (index 2) 16
3.8 Changes of the temperature profile for a feed composition of 30/20/50 . . 17
3.9 Control structure of setup 5 / Cascade Control with fixed vapor split, with primary loop (index 1) and secondary loop (index 2) 18
3.10 Control structure of setup 6 / partial Cascade Control, with primary loop (index 1) and secondary loop (index 2) 20

4.1 Steady State 22
4.2 Effects of small changes in feed rate and feed composition (Initial model) 22
4.3 Major changes of the Feed rate: 130 % (Initial model) 23
4.4 Major changes of the feed composition (Initial model) 23
4.5 Comparison of the initial model and Setup 2 for a decreased feed rate of 70 % 24
4.6 Comparison of the initial model and Setup 2 for a feed composition of 50/20/30) 25
4.7 Smaller and shorter deflection with temperature control (Feed rate 70 %) 25
4.8 Temperature control reacts faster, but does not meet the concentrations setpoints for minor variations in the feed composition (Feed composition 30/40/30) 26

4.9 In Temperature Control, major changes in the feed composition cause large deflections and violations of the constraints 26
4.10 With Cascade Control, the requested purities can be reached for most of the changes in the feed compositions (Here: Feed composition 40/40/20) . 27
4.11 High fractions of component A causes errors in the Cascade control (Here: Feed composition 50/30/20) 28
4.12 Example of Overshoot in Setup 5, caused by growing I-part of not active controller VB2 28
4.13 The partial cascade control is slower than pure temperature control for changes in the feed rate (decreased feed rate of 70 %) 29
4.14 The final Setup meets all constraints for cases where previous layouts fail (e.g. for composition 30/50/20) 30

1 Introduction

The separation of several products is a common task in chemical processes. For many liquid components, continuous distillation is a good choice. But if the feed contains more than two different components, another column has to be added for every further component and the investment costs rise. Furthermore the separation problem becomes more and more complex as the possible combinations of the different columns increase. For a mixture of only three substances (A, B and C), one can for example use a direct or indirect sequence. Another possibility would be a setup with a small prefractionator where A and C are split and a main column for the more difficult A/B and B/C splits.

A major improvement comes with the thermally and mass-coupled setup introduced by Petlyuk et al. [2], where a prefractionator and a main column are connected so that mass streams flow in both directions. With this setup only one condenser and one reboiler is needed for the hole setup (see figure 1.1). Compared to a sequential setup, this structure can save up to 25 % investment costs and 35 % energy costs [6].

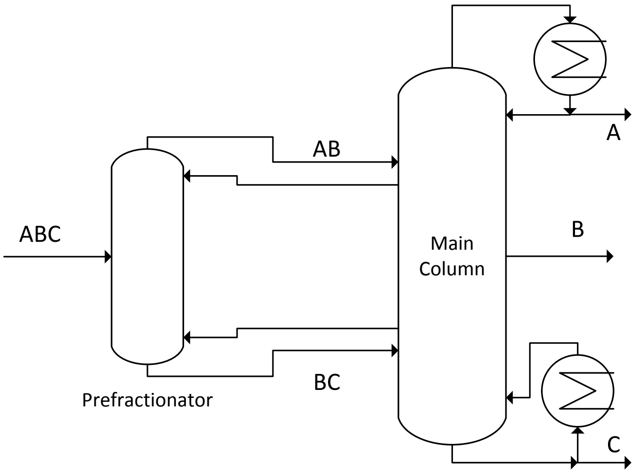


Figure 1.1: Thermally and mass-coupled setup according to Petlyuk

Still there are only view columns of this type in industrial use. The downsides of this structure are the difficulties in controlling and operating which often outweigh the benefits. Especially in processes where conditions change frequently, the large number of degrees of freedom can become a problem.

This work compares different control structures like composition control, temperature control and full cascade control as well as partial cascade control for a Petlyuk like three-product column. The aim is to find a control structure with a good response to dynamic disturbances in the feed. At the same time, the effort for tuning should be manageable.

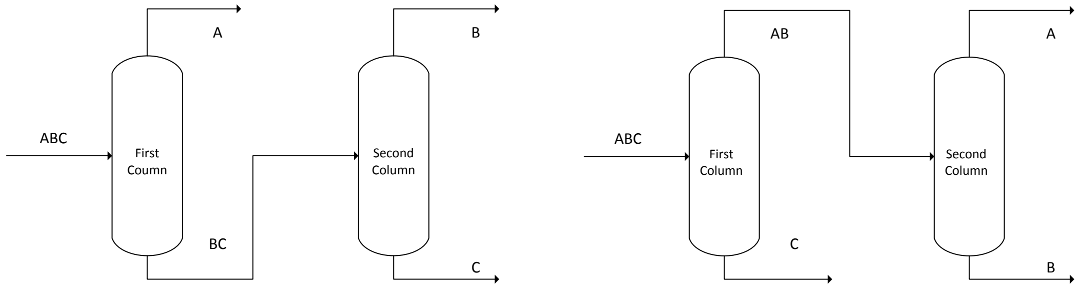
2 Theory

2.1 Petlyuk Column

The straightforward method to distillate a mixture of three components (A, B and C, where A is the light component and C the heavy one) is the use of a direct or indirect sequence (see figure 2.1). Depending on the difficulty of the Split A/B and B/C and the fractions of the three components, the more suitable and economic method can be chosen. In every setting a large first column is needed to achieve a sharp split of two of the substances. Simultaneously the third fraction has a part in the mass flows and therefore requires bigger dimensions of the equipment, but is not purified in this section.

Another better possibility would be a setup with a prefractionator (see figure 2.2a on the following page) in which the easy split between A and C takes place in a smaller first column (the prefractionator) and the more difficult A/B and B/C splits are handled in the main column. In this setup every section has only to be big enough to hold the components that are actually separated in this section. The selection of the best layout depends on the feed composition and many other parameters like energy costs, the interest in investment costs and process details of the separation problem.

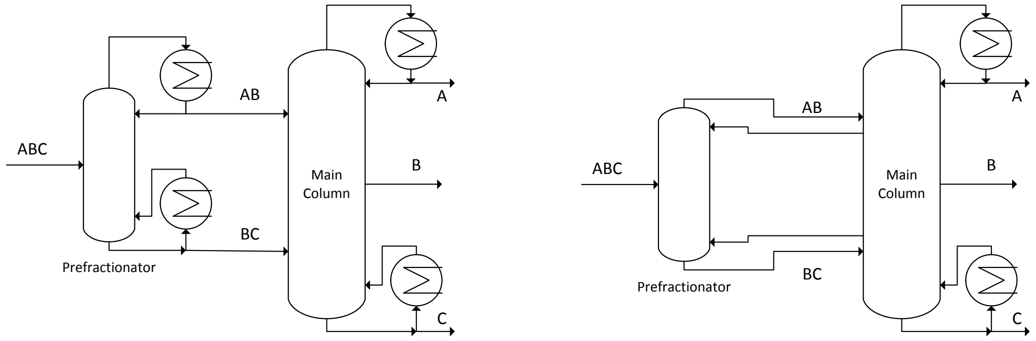
But still each column needs a separate condenser and reboiler. A major improvement comes with the thermally and mass-coupled setup introduced by Petlyuk et al. [2], where the prefractionator and the main column are connected in both directions (see figure 2.2b on the next page). Therefore parts of the liquid coming down from the main column can be used as reflux in the top of the prefractionator and the steam going up can replace the boil up in the small column. So with this setup only one condenser and one reboiler



(a) Direct Sequence

(b) Indirect Sequence

Figure 2.1: Direct and indirect sequence to separate a mixture of the three components A, B and C (Condensers and reboilers are not shown)



(a) Setup with Prefractionator

(b) Thermally and mass-coupled setup according to Petlyuk

Figure 2.2: More advanced structures to separate three components A, B and C

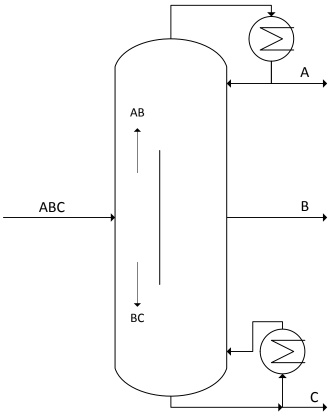


Figure 2.3: Combination of the prefractionator and the main column into one divided wall column

is needed for the hole setup and the investment costs as well as the energy consumption can be reduced significantly.

A further step to save material and space is the combination of the prefractionator and the main column in one single column, a *divided wall column*. An internal wall separates the feed stage from the stage of the side product and prevents remixing (see figure 2.3). Compared to a sequential setup, this structure can save up to 25 % of investment costs, 35 % of energy costs and 40 % of pace [6]. Even the additional costs for the wall inside are compensated by saving a complete column and most of the external piping.

Nevertheless, only a few of these Petlyuk and divided-wall columns have been built. The disadvantage of this structure is the increased number of degrees of freedom. As a result both the design and the controlling become more complex and the whole structure gets difficult to built and to handle.

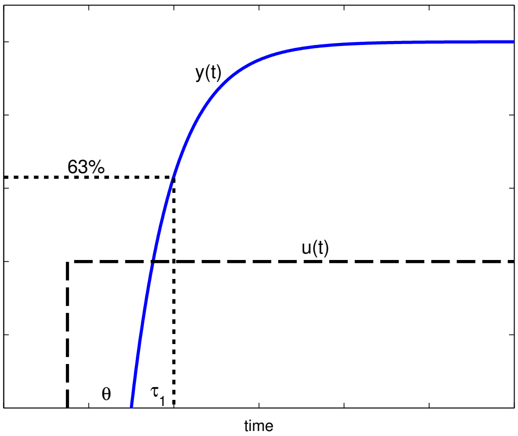


Figure 2.4: Step response to a change of the controlled value u(t)

2.2 Controller Tuning Rules

Besides the correct pairing of inputs and outputs, one of the main tasks in accomplishing a good control structure is the tuning of the controllers. Especially for a complex setup like the divided wall column, a systematic procedure is needed to find well working settings. In this work, all PI controllers are tuned using the SIMC tuning rules as described by Skogestad [4].

2.2.1 SIMC tuning rules

The procedure according to Skogestad would be to first obtain a first or second order model of the control problem and then to derive the controller settings following the SIMC rules. In case of the divided wall column, probably a higher order model would be needed to sufficiently represent the actual column. Nevertheless, as the whole column already is a MATLAB model, the faster method is to examine the response of the system to step changes in the manipulated variables.

Based on the steady state, a small step change of a controlled value ($u(t)$, in this case the flow rates in the valves) is made for each valve separately. After a time delay θ, the corresponding measured value ($y(t)$, here the compositions) will change and settle at a new level (see figure 2.4). For the tuning rules, several parameters of the step response have to be measured. The effective time delay θ (the time between the step in $u(t)$ and the first response of $y(t)$, also known as dead time), the dominant lag time constant τ_1 (the time the measured value takes to reach $63\,\%$ of its maximum; starting after the dead time) and the steady state gain k (which is defined as the ratio of the response amplitude and the step size).

$$k = \frac{\Delta y_\infty}{\Delta u} \tag{2.1}$$

Furthermore, the closed-loop time constant τ_c is used as a tuning parameter to tighten (higher τ_c) or de-tune (lower τ_c) each controller. A good initial value can be $\tau_c = \theta$, which results in a good compromise between speed, stability and robustness.

If the lag time is much bigger than the time delay ($\tau_1 > 8 \cdot \theta$), the first order response can be approximated by an integrating process. Instead of the the gain k, the value of k' is then used for the tuning, where k$'$ is the slope of the approximated linear response divided by the step size.

$$k' = \frac{\Delta y / \Delta t}{\Delta u} \tag{2.2}$$

In practice, the time period in which the slope is measured, should be about the same size as the used τ_c. If θ is very small and the integrating approximation is used, the SIMC rules result in $\tau_\mathrm{c} = \theta \approx 0$ and τ_c has to be set to an adequate value bigger than zero.

Based on these values, the controller settings can be calculated as follows

	First Order	Integrating
Controller gain:	$K_\mathrm{c} = \frac{1}{k} \cdot \frac{\tau_1}{\tau_\mathrm{c} + \theta}$	$K_\mathrm{c} = \frac{1}{k'} \cdot \frac{1}{\tau_\mathrm{c} + \theta}$
Integration time constant:	$\tau_\mathrm{I} = min\left[\tau_1, 4 \cdot (\tau_\mathrm{c} + \theta)\right]$	$\tau_\mathrm{I} = 4 \cdot (\tau_\mathrm{c} + \theta)$

2.2.2 Tuning procedure

The dynamic response of a distillation column is strongly nonlinear and therefore is harder to handle the further the current operation point is away from the nominal value. The use of a logarithmic composition instead of the pure concentrations is sufficient to counteract most of this non-linearity. So the measured value for every controller $y(t)$ is actually $\ln(x_i(t))$ and the setpoint is $\ln(x_i(0))$. [3]

The procedure for all control structures is to tune the controllers in the prefractionator independently at first, while all other loops are open. Then these two loops are closed and the remaining controllers in the main column are tuned one by one, while the other loops in the main column stay open. After all parameters are obtained and all control loops are closed, usually the boil up and the reflux have to be de-tuned as they most likely interact.

3 Simulation Models

Starting with an existing MATLAB model of a Petlyuk column, different setups are implemented. The originally used composition control is first changed to temperature control and then to cascade control.

3.1 Basics of the MATLAB model and steady state

The core of the program is based on *column A* as it is introduced by Skogestad and Morari [5] and used in several of their papers (e.g. [3]). While *column A* only works on binary mixtures, the expansion to three and four product separation was done by the Distillation Group of Sigurd Skogestad at NTNU. As the key aspect of this studies is the controlling and not the column design, some assumptions are made to get an easier model. This allows to focus on the control structure without having to care about the effects of non-ideal mixtures which are in most cases small but time-consuming to calculate.

The properties of the theoretical components A, B and C are close to a mixture of ethanol, propanol and n-butanol. The pressure in the column and the relative volatilities are assumed as constant. Moreover, constant internal molar flows in each section, a total equilibrium on all stages and a total condenser are used. While the flow dynamics of the vapor are neglected, the liquid dynamics are approximated by a linear model. The parameters of the column are summarized in table 3.1.

In this model, three single columns are used to represent the divided wall column (see figure 3.1 on the next page). In terms of controlling and thermodynamics, this setup is equivalent to an actual divided wall setup. Each column consist of two sections with 20 theoretical stages in each section. The first column (section 1 and 2) works as the prefractionator and the other two (section 21 to 24) form the main column. In the main column, there are also the three stages top, S1 and reboiler which represent the condenser, the stage where the side stream is branched off and the reboiler. In order

Table 3.1: Parameters of the model

Relative volatilities [A B C]	[4.2 2.1 1]
Stages in prefractionator	2 x 20
Stages in main column	4 x 20
Feed rate	1 kmol/min
Feed composition	equimolar
Feed state	saturated liquid

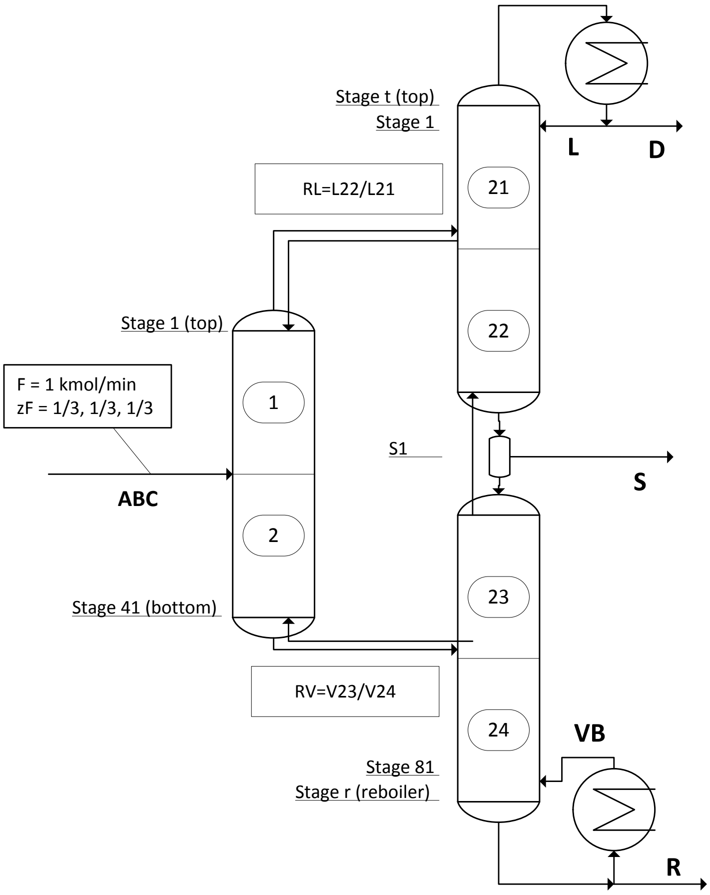


Figure 3.1: Implementation of the Petlyuk structure

Table 3.2: Steady state values

column	main				prefractionator	
position	distillate	residue	side	product	top	bottom
nominal impurity [mol %]	0.5	0.5	0.5	0.05	0.29	0.08
by component	B	B	C	A	C	A

Table 3.3: Nominal Flow rates

Stream	L	VB	RL	RV	S	D	R
nominal flow [kmol/min]	1.0034	1.3382	0.6535	0.4019	0.3318	0.3348	0.3333

to prevent confusion between the component B and the bottom product, the bottom product is called residue (R) in the following. In all cases a *LV-configuration* is used. The two external flows in the top and bottom (D and R) are used to control the liquid hold-up in the condenser and the reboiler. This leaves five degrees of freedom to control the concentration profiles within the columns. The liquid reflux (L) and the vapor boil-up (VB) are typically used to control the composition in the main column. The prefractionator can be controlled by the ratio of vapor and liquid that is returned from the main column. The vapor split is defined as the percentage of vapor which rises in the upper parts of the main column (R_L = vapor $\text{flow}_{\text{section 23}}$/vapor flow $_{\text{section24}}$). Accordingly, the liquid split is the percentage of liquid that flows into the lower parts of the main column (V_L = liquid $\text{flow}_{\text{section 22}}$/liquid flow $_{\text{section21}}$). With the side stream (S), the middle part of the main column can be controlled.

Based on a steady state, the effects of step changes in the feed rate and the feed composition are tested. The steady state is adopted from earlier work of Dwivedi et al. [1], who used this state close to minimal energy consumption. The nominal key impurities (table 3.2) and related controller settings (table 3.3) are shown above.

Dwivedi et al. [1] also showed that in terms of energy consumption and controlling it is suitable to over-purify the streams in the bottom and top of the prefractionator

3.2 Control Structures

For all simulations, variations of a L-V-configuration are used where the reflux (L) and boil up (VB) control the compositions in top and bottom of the main column.

3.2.1 Initial Control Structure (Setup 1)

In the initial setup, the simplest control structure is used. While it is comparatively easy to implement this setting, the system is very sensitive to changes in the feed rate and the feed composition.

Table 3.4: Initial controller pairing and tuning parameters

Controller	L	VB	S	none	RL	RV	D	R
key component	B	B	C	A	C	A	liquid level	
column	main				prefractionator		main	
position	distillate	residue	side product		top	bottom	condenser	reboiler
τ_c	6	15	5		25	30		
K_c	0.339	0.139	-0.557		-0.109	-0.033	1	1
τ_I	45	70	28		100	120	1000	1000

In addition to the reflux and boil up, the liquid split (R_L) and vapor split (R_V) are used to control the compositions in the top and the bottom of the prefractionator. The side stream (S) controls the composition of the side product. In this initial case, only the impurity of component C in the side stream is controlled (see also table 3.4 and figure 3.2 on the next page).

Initially the approach for the best tuning was to first set the prefractionator and then to try to tune the main column accordingly. It was assumed that a tightly tuned prefractionator would stabilize the whole system. But with a tight controlling in the prefractionator, the mass flows going into the main column start to fluctuate very fast. While the many stages of the main column can handle small deflections in the composition well, changes in the flow rates disturb all the controllers. Therefore it is recommended to tune the small column at least about the factor 5 slower than the big one.

3.2.2 Setup 2: Control of side stream purity with boil-up

The uncontrolled concentration of component A in the side stream can cause impurities in the side product for certain feed compositions. As the attempt to control both components A and B in the side stream by the controller *S1* leads to poor dynamic behavior [1], a second criterion for the boil up is added. Therefore, the controller *VB* is split into two parts *VBB1* and *VBB2*. While *VBB2* is the known part depending on the concentration of component B in the reboiler, *VBB1* controls the concentration of A in the side stream. The boil up is coupled to a maximum selector which transmits the bigger of the two values (see figure 3.3 on page 12). The new parameters are shown in table 3.5 on the next page. Due to the maximum selection, single product streams may be over-purified in some cases, but then all purity constraints are met in the new states.

3.2.3 Setup 3: Temperature control

A further step to improve the performance of the column is to use temperature control. In practice it is easier to measure the temperature in the column than to measure the composition. A temperature sensor works continuously and very fast. Measuring the concentration can be done with an gas chromatograph and can take up to 15 minutes for

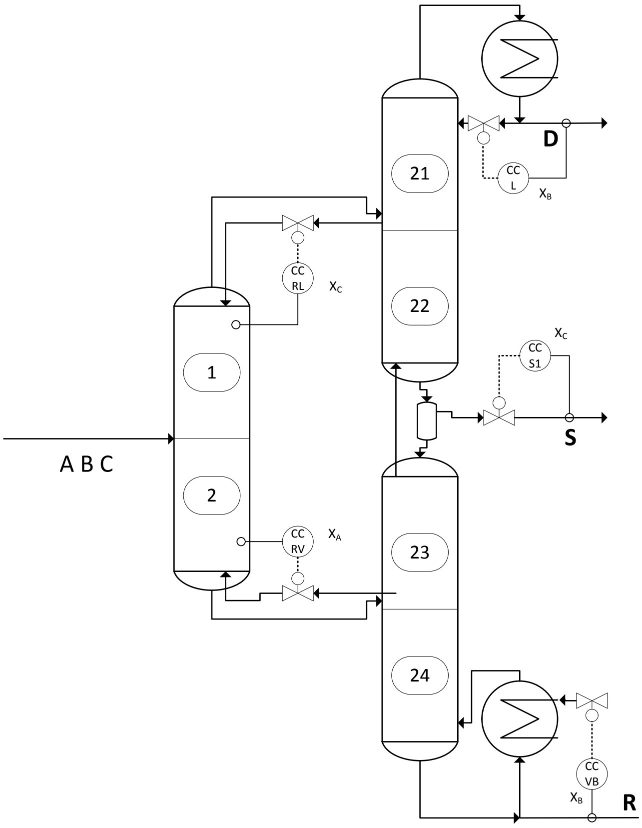


Figure 3.2: Control structure of setup 1

Table 3.5: Controller pairing and tuning parameters of Setup 2

Controller	L	VB2	S	VB1	RL	RV
key component	B	B	C	A	C	A
column	main				prefractionator	
position	distillate	residue	side product		top	bottom
τ_c	6	15	5	19	25	30
K_c	0.339	0.139	-0.557	0.1	-0.109	-0.033
τ_I	45	70	28	80	100	120

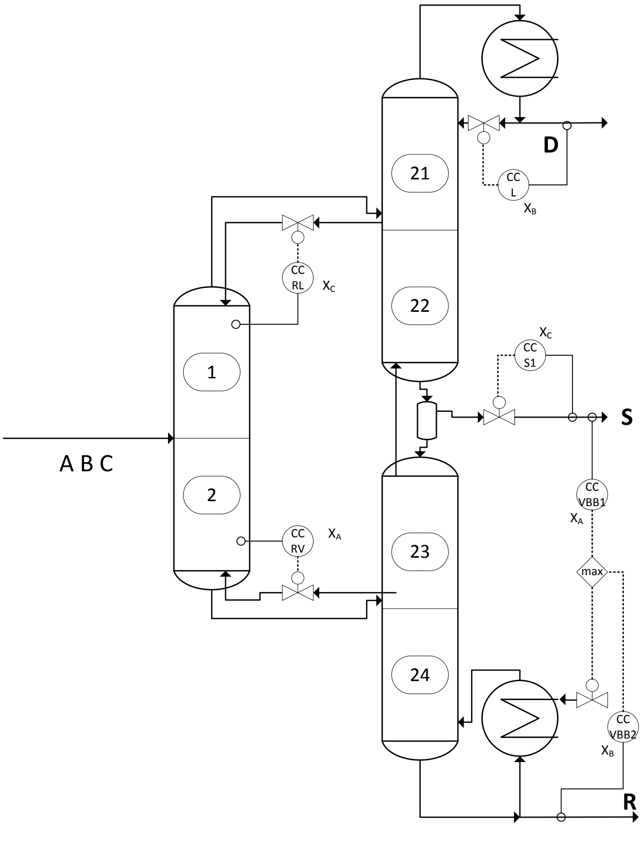


Figure 3.3: Control structure of setup 2

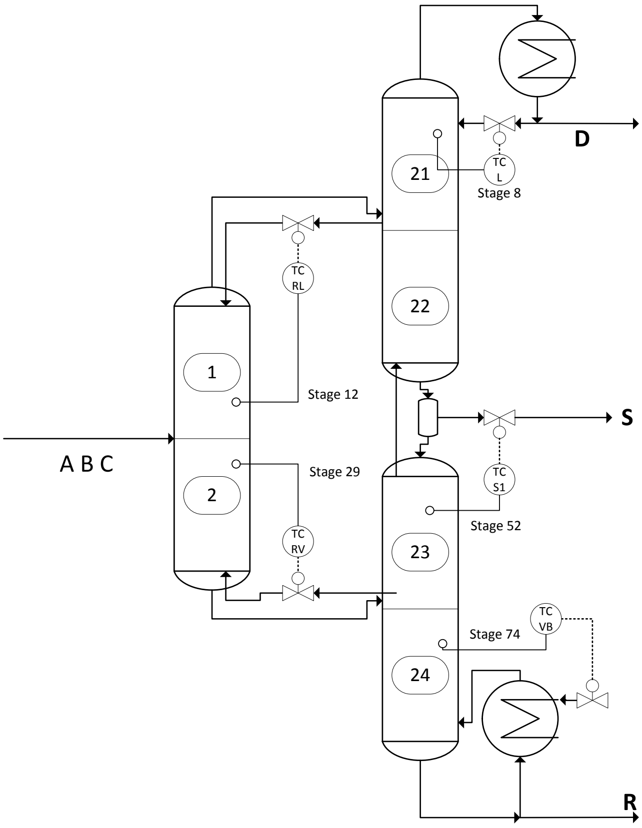


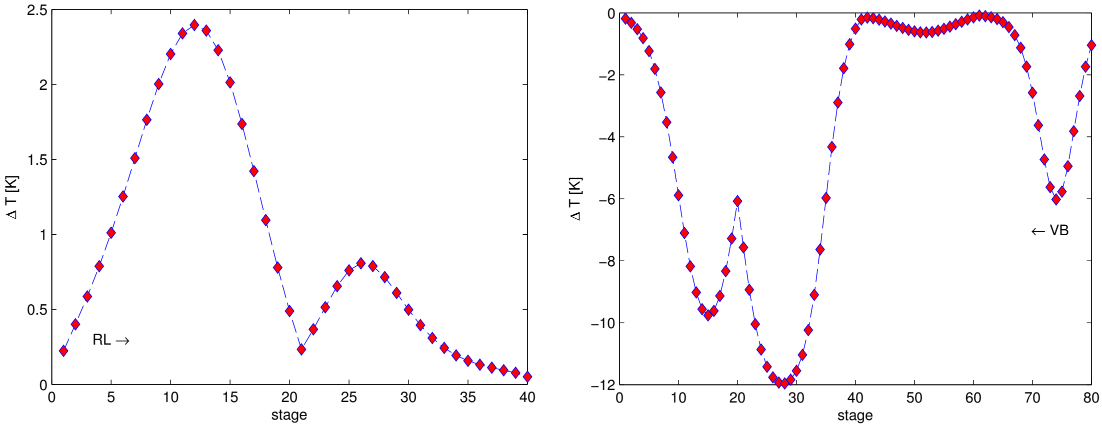
Figure 3.4: Control structure of setup 3 / Temperature Control

one measurement. Temperature control also brings some additional advantages. As the temperature is not measured at the end of the column but around the middle of a section (see figure 3.4), changes can be detected much earlier and the controller is able to respond to disturbances before they even reach the product streams. Therefore, the whole column profile is stabilized and the sensitivity to disturbances is reduced. Furthermore there is no need to split the boil up controller when using temperature control. Instead of one controller for each the concentration of A and C in the side stream, the monitored temperature is dependent of both concentrations.

For this simulation, the liquid phase is assumed as an ideal mixture and the temperature is approximated by an linear weighting of the boiling temperatures of the three components with their mole fraction.

$$T \approx \sum_i x_i \cdot T_i \tag{3.1}$$

To decide at which stage the temperature should be controlled, the stage with the highest steady-state gain has to be found for each controller. Therefore, all control loops are opened (except the level controllers D and B) and the changes of the temperatures of each stage are plotted for a certain change of the controller value. In most cases, you



(a) Prefractionator, increased *RL* of +0.01 (b) Main column, decreased *VB* of -0.01

Figure 3.5: Temperature changes in the prefractionator and the main column for changed controller values

would expect graphs like the one in figure 3.5a. There should be no or only a small change in the temperature at the ends of the column and a maximum around the middle of the section closest to the changed flow. Normally you would choose the stage with the highest temperature change as control point (stage 12 for RL) and tune the controller according to the SIMC-rules (see section 2.2). A logarithmic temperature is not used in these simulations.

However, the effects of the position must always be taken into account. The highest gain in figure 3.5b is obviously at stage 28. But regarding the liquid flow dynamics and the outlet *S1* between the control point and the controller, this setting would be difficult to handle and the performance would be slow. So for this case it seems more reasonable to choose stage 74, which has a lower gain but is much closer to the controller.

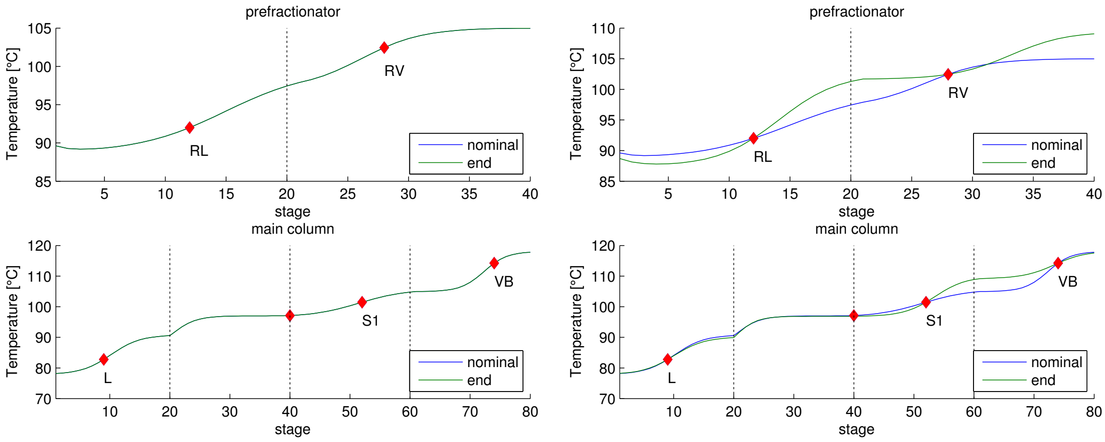
A similar scenario occurs for the controller *S1* (no figure). The stage with the highest temperature change is above the outlet of the side stream. As the side stream branches off the liquid flow, only the section below is affected directly. The changes in the section above are caused indirectly by the increasing boil-up. To avoid this complex connection, the stage with the second highest gain is chosen. This one is below the side stream and can be affected directly by the controller.

The determined stages for all controllers, the controller settings and the corresponding nominal temperatures can be seen in table 3.6 on the facing page.

While temperature control is a good choice for changing feed rates, its fails for changes in the feed composition. The source of this problem lies in the nature of the temperature control itself. A different feed rate requires a proportional adjustment of all controllers and does not change the temperature profile in the column (figure 3.6a on the next page). The temperature control can handle this variations very good, because it already reacts when the changes reach the measure points and not only after the product purity

Table 3.6: Stages and nominal values for the temperature control (Setup 3)

Controller	L	VB	S	RL	RV
column	main			prefractionator	
Section	21	24	23	1	2
Stage	8	74	50	12	28
Nominal Temperature	81.6 °C	114.2 °C	100.3 °C	92.0 °C	102.5 °C
τ_c	1	1	0.5	5	5
K_c	0.477	−0.564	−1.459	−0.282	−0.125
τ_I	6.7	4	4.8	23	20



(a) Feed-rate 130 %

(b) Feed composition 30/20/50

Figure 3.6: The temperature profile does not change for feed rate variations, while changes in the feed composition have an obvious effect on it

drops. In contrast to this, a change in the feed composition has a strong effect on the temperature profile (see figure 3.6b). So even if the controllers manage to hold the temperatures at the different measurement points, the constraints for the products may be violated. In order to deal with the changing demands on the temperatures for different feed composition, a cascade control is needed which also considers the product purities.

3.2.4 Setup 4: Cascade Control

The results from section 3.2.3 show that changes in the feed composition implicate the need to adjust the setpoints of the temperature control. Therefore a second control loop (primary loop) is added to the previous model. This new control layer changes the temperature setpoints according to the concentrations of the key-components in the column (see figure 3.7 on the next page). The present temperature control (secondary loop) is tuned tight and stabilizes the temperature profile over the complete column

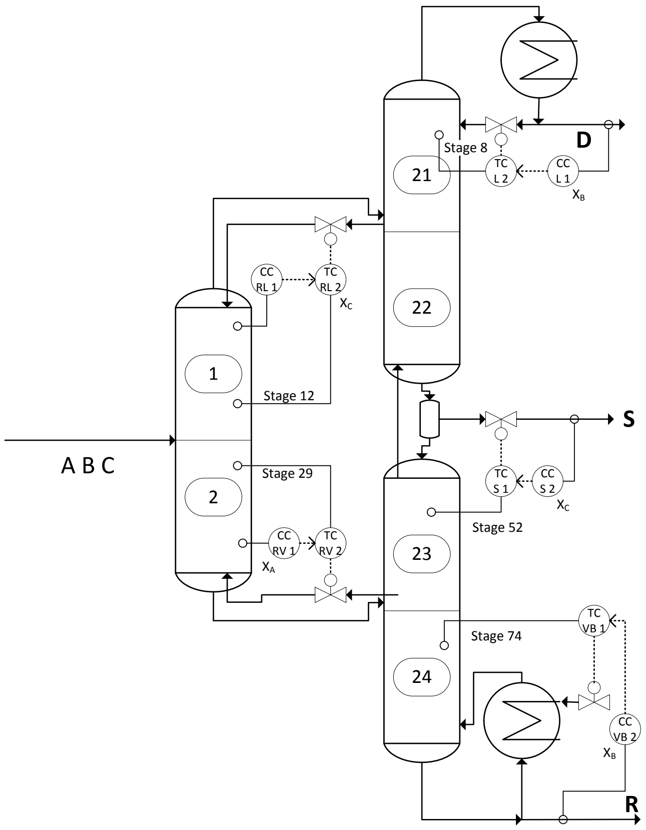


Figure 3.7: Control structure of setup 4 / Cascade Control, with primary loop (index 1) and secondary loop (index 2)

Table 3.7: Tuning parameters of the cascade control (Setup 4)

Controller		L	VB	S	RL	RV
primary loop	τ_c	10	15	5	10	15
	K_c	−4.98	2.51	−0.323	−0.693	0.748
	τ_I	43	60	5	40	60
secondary loop	τ_c	2	2	0.5	5	5
	K_c	0.341	−0.282	−1.49	−0.286	0.125
	τ_I	10	8	4.68	22.8	20

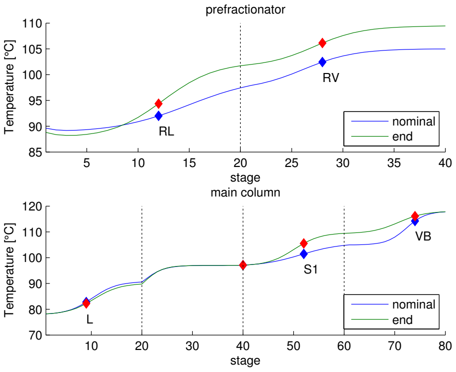


Figure 3.8: Changes of the temperature profile for a feed composition of 30/20/50

very fast. The primary loop can be tuned slower and only adjusts the temperature setpoints so that the concentration constraints in the product streams are met. In order to prevent an interference between the two control layers, their speed, respectively the tuning parameters τ_c should differ at least by the order of five to ten. The used controller parameters are shown in table 3.7. In contrast to setup 2, the uncontrolled concentration of component A in the side stream is not a problem in this setup. Apparently, the three controlled temperatures are sufficient to stabilize the whole column profile. Anyway, none of the controllers has a direct influence on the concentration of A in this stream.

This combined control structure results in a changed temperature profile (see figure 3.8), but the product streams comply better with the specifications than with pure temperature control.

3.2.5 Setup 5: Cascade Control with fixed Vapor Split

In addition to some control problem of Setup 4 (see section 4.4), a variable vapor split is also complicated to implement structurally. Any use of a valve would cause changes in the pressure drop of both parts of the column and make the already complex control structure even more difficult. Thus the most common way is to use a fixed vapor split. To be able to control the state in the bottom part of the prefractionator anyway, a second criterion can be added to the boil up controller. For this setup, the part VB3 is added.

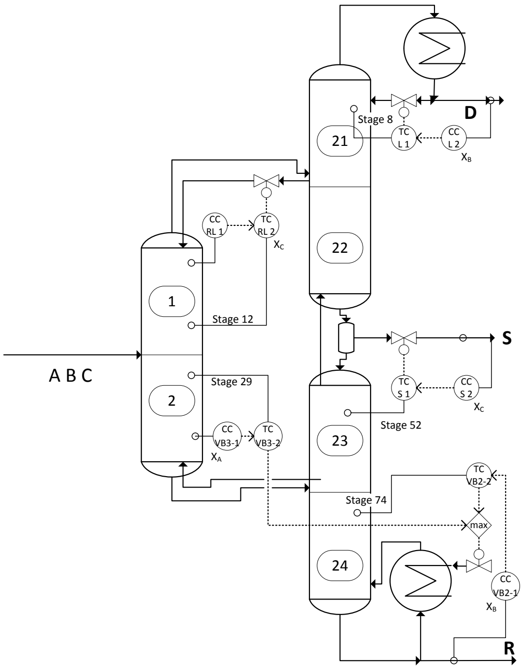


Figure 3.9: Control structure of setup 5 / Cascade Control with fixed vapor split, with primary loop (index 1) and secondary loop (index 2)

It monitors the same stage and temperature as the former controller RV, but instead of the vapor split, now it changes the boil up (see figure 3.9). Similar to the part VB1 in section 3.2.2, the two criterions (VB2 and VB3) are coupled with a maximum selector and the boil up is adjusted to the bigger value. The vapor split is fixed to the nominal value of 0.4. The tuning parameters for the other controllers stay basically the same as for Setup 4. The values for the new part VB3 are shown in table 3.8.

Table 3.8: Tuning parameters of the cascade control with fixed vapor split (Setup 5)

Controller		L	VB2	S	RL	VB3 (RV)
primary loop	τ_c	10	15	5	10	10
	K_c	−4.98	2.51	−0.323	−0.699	0.732
	τ_I	44	60	5	40	40
secondary loop	τ_c	2	2	0.5	5	5
	K_c	0.341	−0.279	−1.49	−0.286	−0.267
	τ_I	10	8	4.68	22.8	20

Table 3.9: Tuning parameters of the partial cascade control with fixed vapor split(Setup 6)

Controller		L	VB2	S	RL	VB3 (RV)
primary loop	τ_{c}	10	5	5	10	10
	K_{c}	-4.98	0.331	-0.323	-0.699	0.202
	τ_{I}	44	30	5	40	40
secondary loop	τ_{c}	2	-	0.5	5	-
	K_{c}	0.341	-	-1.49	-0.286	-
	τ_{I}	10	-	4.68	22.8	-

3.2.6 Setup 6: Partial Cascade Control

Besides the mentioned issues, the control structures introduced as Setup 4 and Setup 5 work quite well for many of the tested cases. As a downside, the tuning of their controllers is not straight forward. The boil up and the reflux are most likely to interfere with each other and start to oscillate easily. In combination with the prefractionator and the side stream, the system gets so complex that any controller might couple with any other one. Once a single controller starts to oscillate, it will drag along the other controllers and disturbances will built up over the whole system. So even if the temperature control is tuned well, it has to be re-tuned after the primary loop is closed. The SIMC rules are a good start for initial tuning parameters, but the final tradeoff between speed and robustness has to be found by trial and error and a stepwise retuning of all controllers in several turns. Slight changes in the parameters of setup 5 can already cause major failures for most feed cases.

An easier approach for a good control structure is a partial cascade control, where only some of the streams are handled by a primary and a secondary loop. In setup 6 the secondary loop (temperature control) for the boil up is removed (see figure 3.10 on the following page). Like in the first two setups, the primary loops of VB2 and VB3 directly control the composition and not the temperature setpoints in this layout. Their tuning parameters are adjusted to a not tight composition control (see table 3.9).

Although the states in the bottom of the prefractionator and the main column are only controlled by a slow composition control, the tight temperature control in the upper parts stabilizes the profiles in the whole column. So the combination of fast temperature control in the upper part and slower composition control in the rest of the columns is sufficient to meet all product specifications.

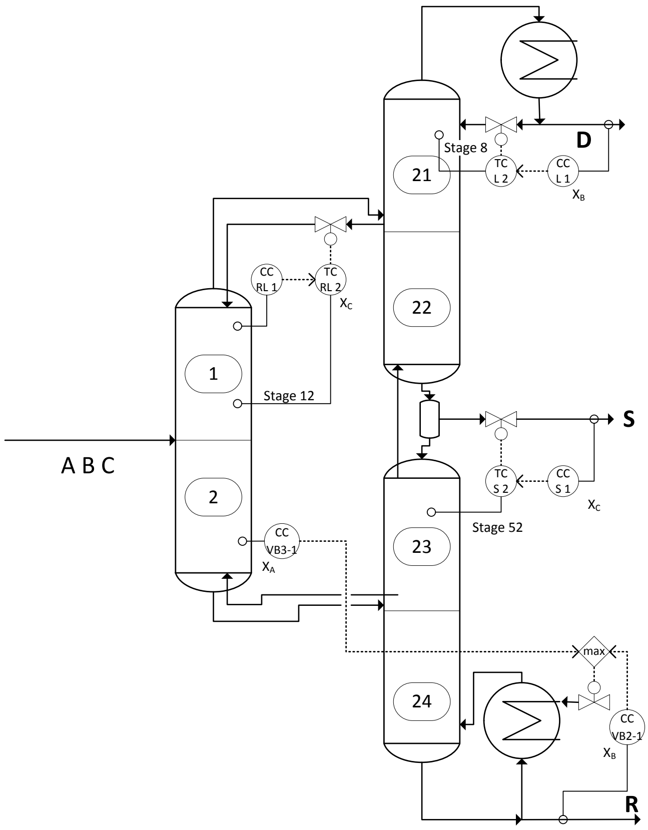


Figure 3.10: Control structure of setup 6 / partial Cascade Control, with primary loop (index 1) and secondary loop (index 2)

4 Results and Discussion

Compared to the steady-state (figure 4.1 on the following page), where the feed rate is 1 kmol/min and the feed composition is equimolar, several simulations with different feed properties are tested in the following. The variations of the feed rate range from −30 % to 30 % in steps of ten percentage points. The short notation is `Fxxx`, where `xxx` is the absolute percentage (for example `F120` for an increased feed rate of 20 %). The feed composition is tested for all possible combinations of mole fractions from 0.2 to 0.5 in steps of 0.1. The different cases are named `xAABBCC`, where `AA` is the molar percentage of the component A, `BB` the percentage of B and `CC` of component C (e.g. `x203050` for 20 % A, 30 % B and 50 % C). Combinations of both rate changes and composition changes are not simulated.

4.1 Initial Control Structure (Setup 1)

The initial control structure is able to deal with slight changes in the feed rate (±10 %) and small changes in the feed composition (see figure 4.2 on the next page). The impurities of the three products show clear deflections, but settle, regarding the size of the column, in a comparatively short time (about 400 min).

For major modifications of the feed properties, the effects are more serious. A variation of the feed rate of 30 % causes a disturbance in the product purity of about 3 percentage points (see figure 4.3b on page 23).

The influence of the feed composition depends very much on fractions of the components. A high concentration of C causes some oscillating during the first 300 min but still results in the defined product purity (see figure 4.4a on page 23). At the same time, a high amount of A in the feed leads to less oscillation, but then the purity of the side streams drops down from 99.45 % to 90.85 %. This is because of the uncontrolled concentration of the component A in the side stream (see figure 4.4b on page 23). In general, this initial setup does not reach the specified product composition for cases with big differences between A and C in the feed.

4.2 Setup 2: Control of side stream purity with boil-up

With this layout, the product purities can be reached for all feed properties that were already tested in the previous section. For an increased feed rate, there is no difference as the critical value for this case is the bottom product purity. But for a decreased feed

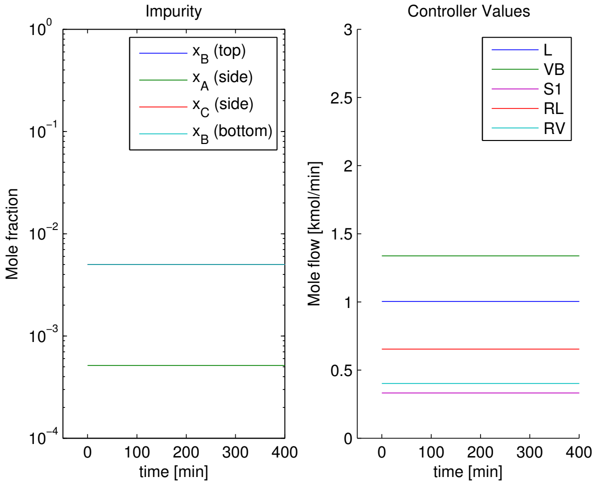
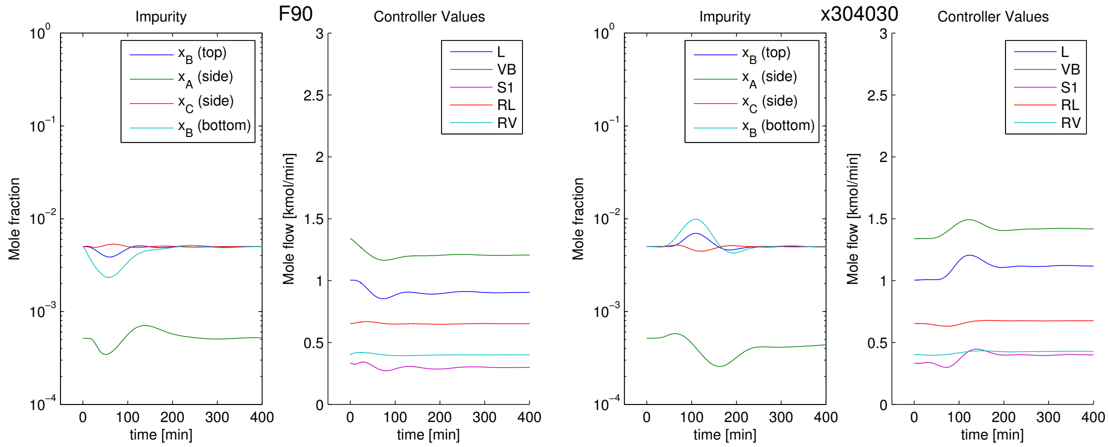


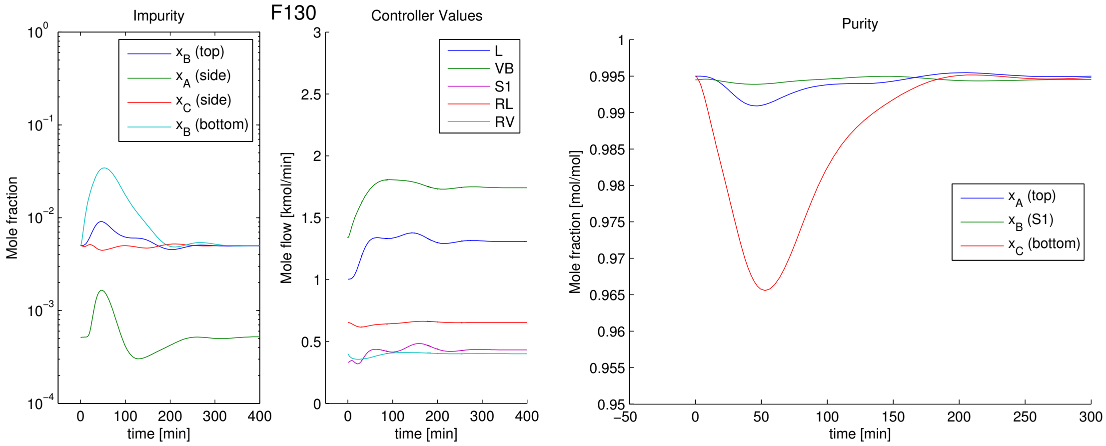
Figure 4.1: Steady State



(a) Feed-rate = 90 %

(b) Feed composition = 30/40/30

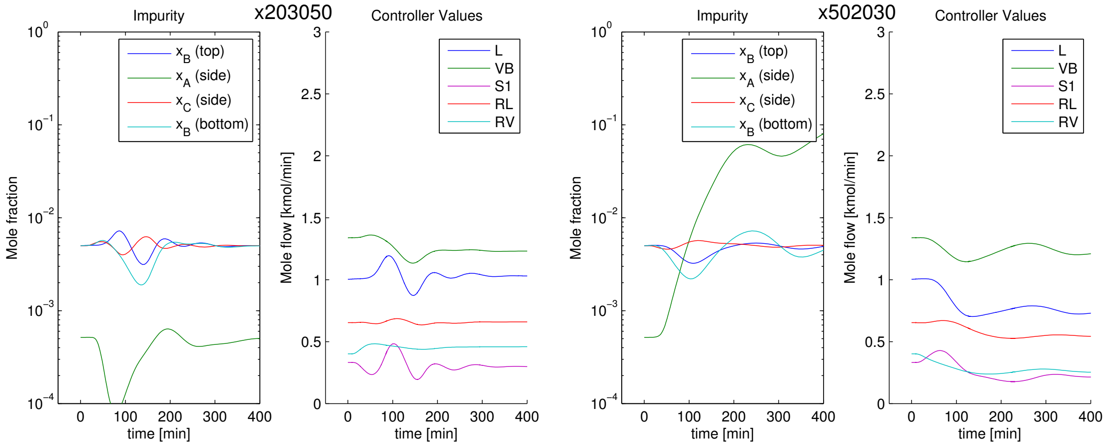
Figure 4.2: Effects of small changes in feed rate and feed composition (Initial model)



(a) Impurities in Product streams

(b) Product Purity

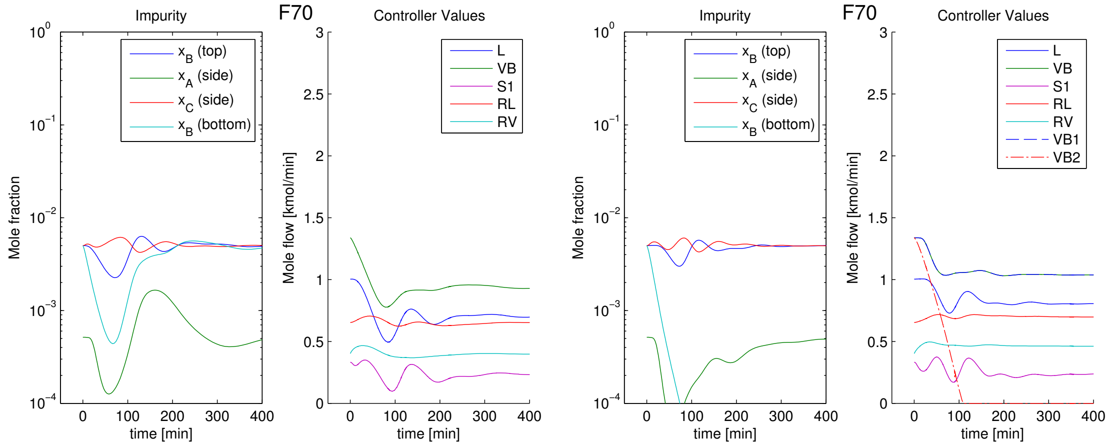
Figure 4.3: Major changes of the Feed rate: 130 % (Initial model)



(a) Feed composition = 20/30/50

(b) Feed composition = 50/20/30

Figure 4.4: Major changes of the feed composition (Initial model)



(a) Initial model

(b) Setup 2

Figure 4.5: Comparison of the initial model and Setup 2 for a decreased feed rate of 70 %

rate, the new part of the controller VBB1 adjusts the concentration of the side product (see figure 4.5).

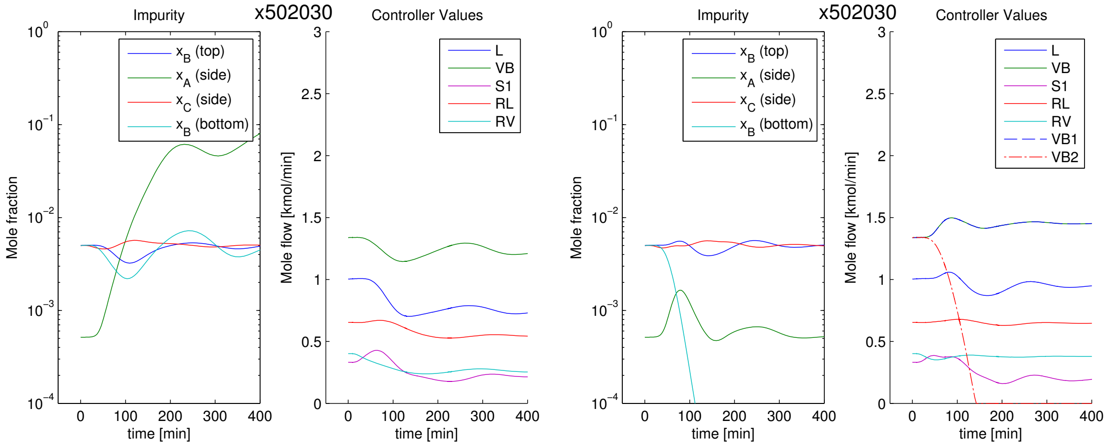
For a variation in the feed composition a similar trend occurs. There is no change in the profiles for a low fraction of A, because the boil up sticks to the part VB2. However, there is an advantage for changes to a low fraction of C in the feed. As shown in figure 4.6 on the facing page, in this cases the maximum selection follows the part VB1 and the increased boil-up results in a sufficient purity of the side stream. The over-purifying of the bottom product is a result of the increased boil-up that has to be accepted in this setup.

4.3 Setup 3: Temperature control

In direct comparison to setup 2, the temperature control shows its strengths and weaknesses. For any changes of the feed rate, the new control structure is superior (see figure 4.7 on the next page). There are hardly any variations in the product purities and the whole system settles at the steady state after only 100 min.

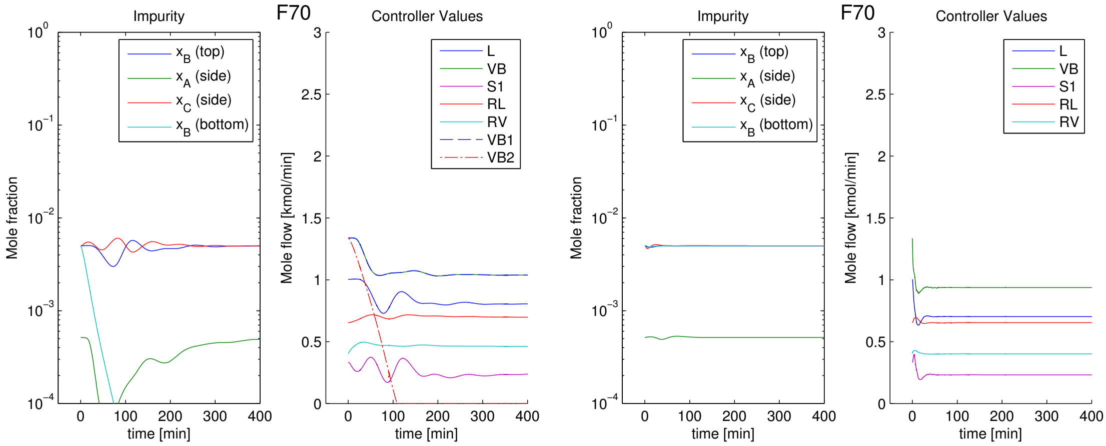
But when it comes to the changes in the feed composition, the temperature control is inferior in almost all cases. It is a bit faster for minor feed changes (see e.g. figure 4.8 on page 26), but already with this small change, the purity constraints are not met. For most of the simulations it does not reach the constraints and shows even larger deflections (see e.g. figure 4.9a and figure 4.9b on page 26).

For a combination of high fractions of the component C and low fractions of A it is not even possible to finish the calculation due to numeric errors of the solver.



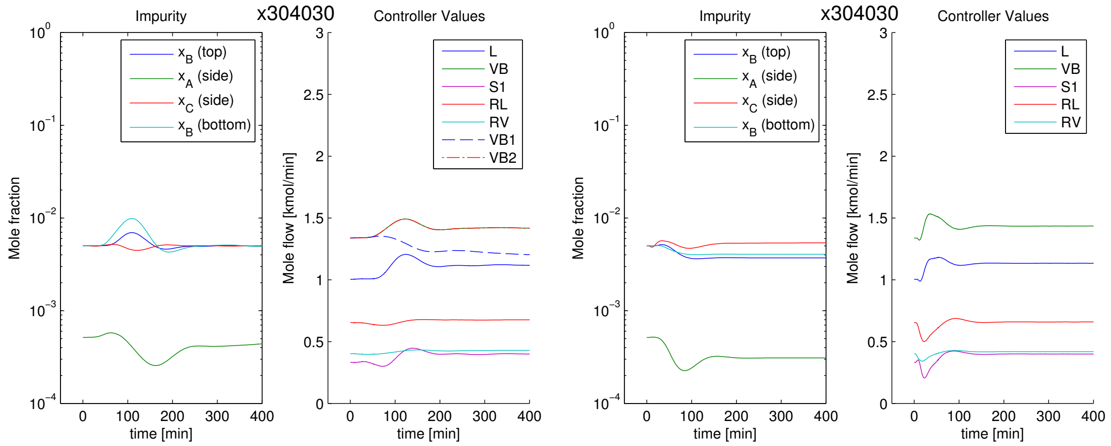
(a) Initial model (b) Setup 2

Figure 4.6: Comparison of the initial model and Setup 2 for a feed composition of 50/20/30)



(a) Setup 2 (b) Temperature control

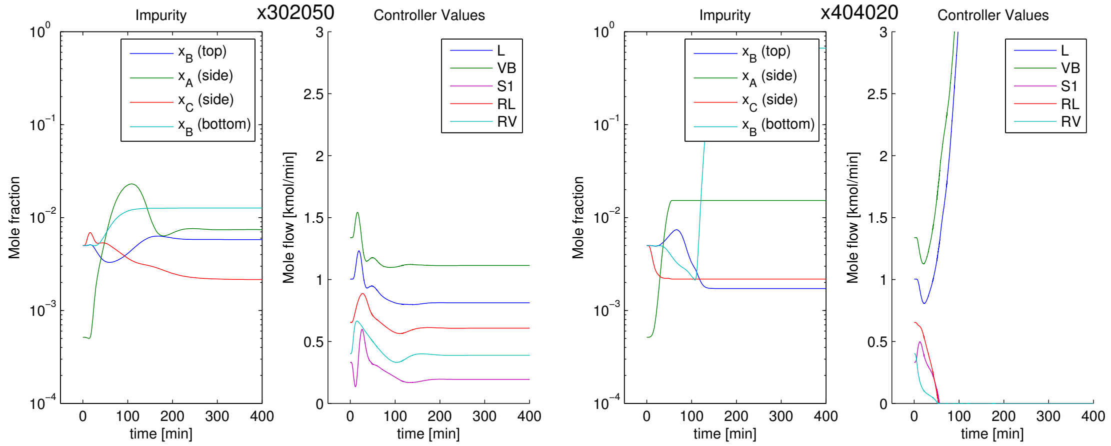
Figure 4.7: Smaller and shorter deflection with temperature control (Feed rate 70 %)



(a) Setup 2

(b) Temperature control

Figure 4.8: Temperature control reacts faster, but does not meet the concentrations setpoints for minor variations in the feed composition (Feed composition 30/40/30)



(a) Feed composition: 30/20/50

(b) Feed composition: 40/40/20

Figure 4.9: In Temperature Control, major changes in the feed composition cause large deflections and violations of the constraints

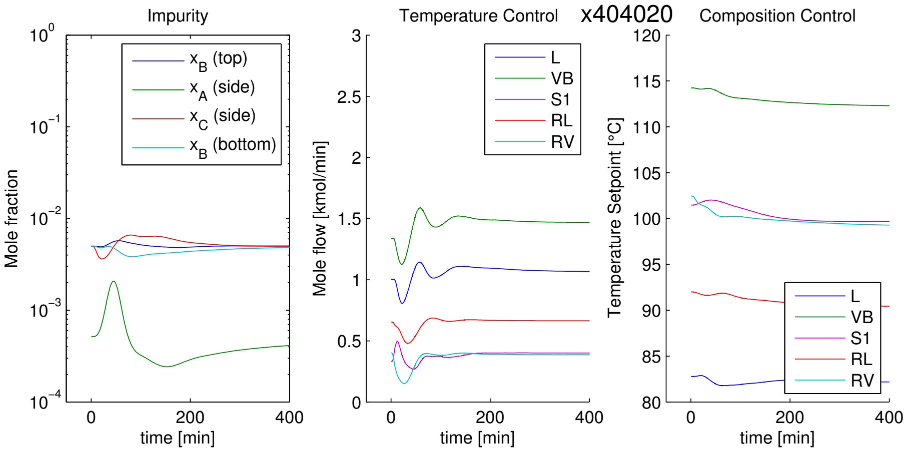


Figure 4.10: With Cascade Control, the requested purities can be reached for most of the changes in the feed compositions (Here: Feed composition 40/40/20)

4.4 Setup 4: Cascade Control

The combination of temperature control and composition control results in a model that works fast and smooth for most of the tested feed settings. For variations in the feed rate it works even a bit faster than the pure temperature control. The major improvement can clearly be seen for variations of the feed composition. While the pure temperature control fails for many settings, the cascade control fulfills the constraints for the product purity in most of the cases (see e.g. figure 4.10).

This Setup is clearly superior to all previous structures, but it still has some weak spots. For a combination of a high fraction of A and a low fraction of C it fails completely (see figure 4.11 on the next page). Due to the too high amount of A in the bottom of the prefractionator, the "boil up" in the prefractionator has to increase respectively the vapor split is changed to 0 by the controller. Therefore, all of the vapor goes through the prefractionator and there is now vapor stream in the main column that can act as counter flow to the liquid stream. So this constellation causes a error in the simulation and obviously would not work in practice either.

4.5 Setup 5: Cascade Control with fixed Vapor Split

The fixed vapor split and the maximum selection for the boil-up solve the problem with the extreme reaction of the RV-controller. At the same time, a new issue occurs. While the boil up is coupled with one of the two controller parts (e.g. VB3) in the beginning, the integrating-part of the non-active controller (here: VB2) still runs. Therefore, the modulus of the I-part of VB2 further increases (see figure 4.12 on the following page). If now the conditions in the column change in a way that VB2 should be active (the concentration of B at the bottom of the column becomes too high at about 150 min), the

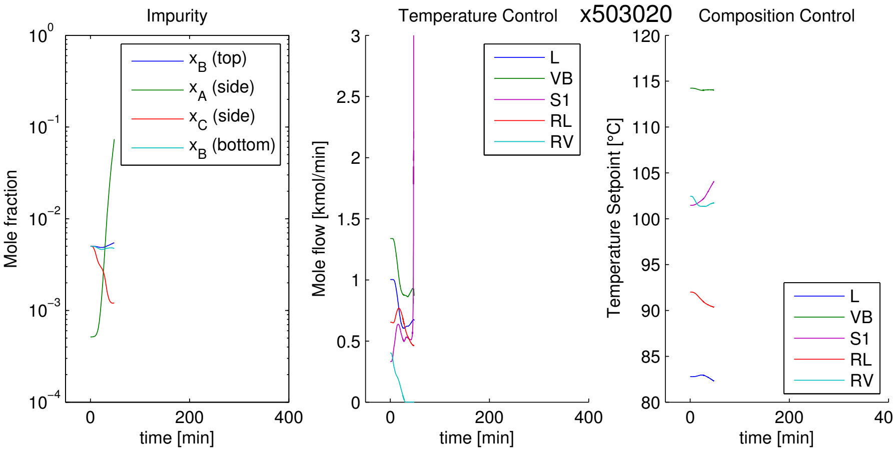


Figure 4.11: High fractions of component A causes errors in the Cascade control (Here: Feed composition 50/30/20)

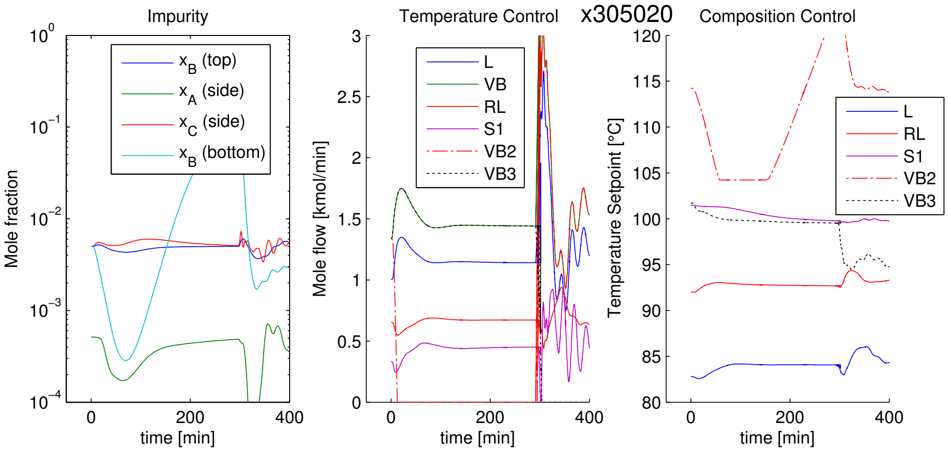


Figure 4.12: Example of Overshoot in Setup 5, caused by growing I-part of not active controller VB2

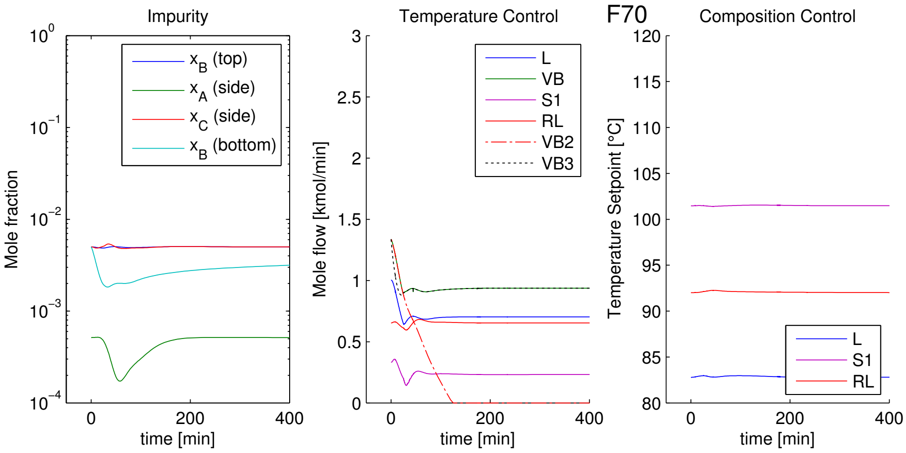


Figure 4.13: The partial cascade control is slower than pure temperature control for changes in the feed rate (decreased feed rate of 70 %)

high remaining I-part causes a dead time of this controller. Once the I-part is decreased and the proportional part is big enough to overcome the I-part, the maximum selector suddenly switches from VB3 to VB2 (here at about 300 min). As the measured error for VB2 is already very high at this point, the sudden change of the controlled stream causes a massive overshoot. Depending on the amplitude of the overshoot the whole system can be disturbed.

There are several solutions to this known problem of the increase of an inactive I-part. The easiest one would be to stop the integration for the non-active controller. But some basic test runs with this implementation are not productive at all. Others are not tested as the problem does no longer exist in Setup 6 (section 4.6).

4.6 Setup 6: Partial Cascade Control

For changes only in the feed rate, this final setup can not compete with pure Temperature control or full Cascade control. Due to the maximum selection there occurs some over-purifying or lag time in the beginning (see figure 4.13). Nevertheless all feed rates can be handled within a reasonable time and without violating the constraints.

On the other hand, there is an advantage for every chase with changes in the feed composition. Here, the partial cascade control can handle every tested scenario. Even in extreme cases like the feed composition of 30/50/20 where Setup 5 completely fails, this control structure is able to meet all constraints and reaches its new steady state within 300 min (see figure 4.14 on the next page).

Any impurities in the product streams and minor oscillations disappear within the first 300 min for all tested feed compositions. Only for a few compositions there is an over-purifying of the side stream that takes longer to resettle to its initial value.

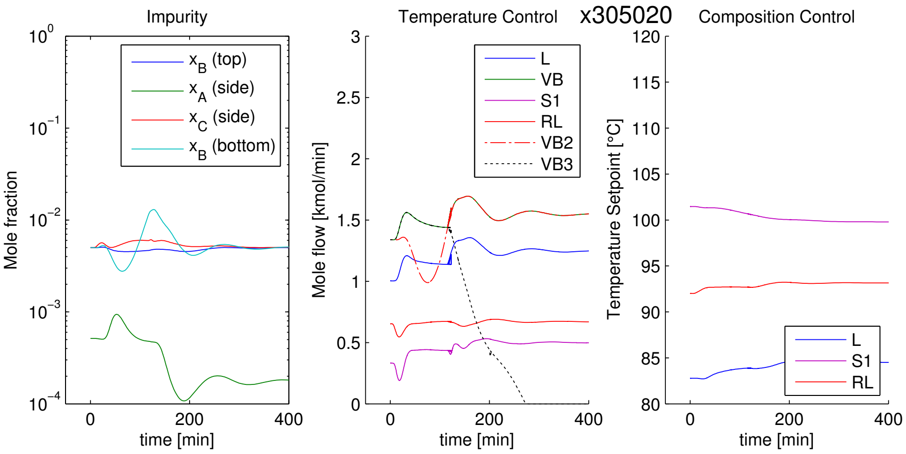


Figure 4.14: The final Setup meets all constraints for cases where previous layouts fail (e.g. for composition 30/50/20)

5 Conclusion

In conclusion, it can be said that the best control structure for a Petlyuk or divided wall column has to be found depending on each process. Setups that are more complex can handle a bigger variety of feed changes. But on the other hand, they are harder to implement and to tune, and can be slower. An overview over the performances of the different control structures is given in table 5.1.

The basic structure, Setup 2 (section 4.2 on page 21), is the easiest one to implement. It can also handle all tested feed scenarios, but the disadvantages are the occurring oscillations and the very slow response to the step changes.
To get a speed boost it is possible to control some feed changes with temperature control (section 4.3 on page 24). While it is much faster for changes in the feed rate the purity requirements are not met for most of the changes in composition.
So especially for processes where the feed composition is unsteady, the temperature control has to be advanced to a cascade control which includes temperature and composition parts (section 4.4 on page 27). This layout copes with minor changes in the feed composition in a reasonable time. Major changes still cause violations in the purity requirements or result in numeric errors. Furthermore, the tuning for a full cascade control is not straight forward and even with the help of methods like the SIMC tuning rules the final controller settings can only be found by many altering changes and a lot of manual work.
Some of the problems can be solved be using a fixed vapor split as in Setup 5 (section 4.5 on page 27). Due to the modifications this model is slower for major feed rate changes. It can handle more but still not all changes in the feed composition. The problems from Setup 4 are eliminated by the fixed vapor split, but new problems emerge simultaneously for some of the cases.
This can finally be solved by opening some of the temperature loops and using a partial

Table 5.1: Performance of the different control structures (−− error, − constraints not reached, *o* constraints slowly reached($>300\,\mathrm{min}$), + constraints reached ($<300\,\mathrm{min}$), ++ constraints quickly reached($<100\,\mathrm{min}$))

	feed changes	feed rate		feed composition		complexity
		±10 %	±30 %	minor	major	
Setup 2	Composition Control	o	o	o	o	low
Setup 3	Temperature Control	++	++	−	−−	low
Setup 4	Cascade Control	++	++	+	− − /o	very high
Setup 5	CC w/ fixed vapor split	++	+	o/+	−/o	high
Setup 6	Partial Cascade Control	+/ + +	+	+	o/+	medium high

cascade control (section 4.6 on page 29). This final setup can deal with all tested scenarios, and is faster than the basic setup. Though the tuning and the control structure is more complicated and it is a bit slower than the full cascade control for changes in only the feed rate.

Anyhow, the effort is manageable by following the SIMC tuning rules. In addition to these tuning rules, it seems, contrary to first thoughts, more practicable to tune the prefractionator looser than the main column.

However, even with the last setup there are still some problems with unnecessary over-purifying of multiple products at the same time. Depending on the process, these variations might still be too big. So for an even more advanced control structure, a model predicted control (MPC) might be necessary. The effort of programming and tuning of a MPC in comparison to the results these controllers can provide, should be considered in further work.

Bibliography

[1] Deeptanshu Dwivedi, Ivar J. Halvorsen, and Sigurd Skogestad. Control structure selection for three-product Petlyuk (dividing-wall) column. *Chemical Engineering and Processing: Process Intensification*, 64:57–67, 2013.

[2] F.B. Petlyuk, V.M. Platonoy, and D.M. Slavinskii. Thermodynamically optimal method for separating multicomponent mixtures. *Int. Chem. Eng.*, 5(3):555–561, 1965.

[3] Sigurd Skogestad. Dynamics and Controll of Distillation Columns: A Tutorial Introduction. *Trabs IChemE*, 75(Part A):539–562, 1997.

[4] Sigurd Skogestad. Simple analytic rules for model reduction and PID controller tuning. *Journal of Process Control*, 13:291–309, 2003.

[5] Sigurd Skogestad and Manfred Morari. Understanding the Dynamic Behavior of Distillation Columns. *Industrial & Engineering Chemistry Research*, 27:1848–1862, 1988.

[6] S. Wenzel and H.-J. Röhm. Auslegung thermisch und stofflich gekoppelter Destillationskolonnen mittels Gesamtkostenoptimierung. *Chemie Ingenieur Technik*, 75(5): 534–540, 2003.