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Influence of Feed Rate on Temperature Controllers in Multicomponent Distillation Columns (in cooperation with Statoil/Gassco at Kårstø)

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Abstract

In this thesis two simulation programs were compared, Unisim and D-spice. This was done by creating a model of three columns in series in Unisim and comparing the dynamic behavior of these models with the models in D-spice. The latter is used by Statoil as a simulation tool. The biggest distinction between the programs is calculation procedure. To make the calculations faster and more robust numerically, D-spice takes advantages of thermodynamical tables, where thermodynamic properties are given for various temperature and pressure, but linearized with respect to composition. Originally, D-spice was doubtless better fitted to the real plant. However, some of the dynamics were found to be more appropriate in Unisim rather than in D-spice. Even though simplicity of column environment and complications in convergence of the solver with more complicated distillation structures was found in Unisim.

Later in this study, control structure was elaborated at lower feed rate, with temperature controllers in priority. It was found that a right operation, that was also found to be the most profitable operation, will not result in critically unstable behavior. Even though the same can not be said about non-profitable operation, gain scheduling was found to be unnecessary tool if process is operated at profitable operation with controllers tuned by SIMC tuning rules.

Finally, optimization, with respect to the cost function of the most energy consumption column at full rate, was executed. The optimization was carried out with regard to impurity fraction of light component in the bottom product, whereas heavy component in the top product was held at two constant values, setpoint for supervisory control layer (Septic) and the specification of stream. The result was somewhat lower impurity fraction of light component bottom than the specification. In fact, J function reduction of 1.6% from specification to optimal operation was found. Consequently, a real time optimization, that would consequently supply control layer below with updated setpoints, was recommended.

Sammendrag

I denne masteroppgaven ble det sammenlignet to simuleringsprogrammer, Unisim og D-Spice. Dette ble gjennomført ved å lage en modell av tre kolonne i serie i Unisim og sammenligne den dynamiske oppførselen av disse modellene med modellene i D-Spice. Sistnevnte er brukt av Statoil som en simuleringsverktøy. Den største forskjellen mellom programmene er måten utregningene blir gjort på. For å gjøre beregningene raskere og mer robuste numerisk, bruker Dspice termodynamiske tabeller der termodynamiske størrelser er gitt for ulike temperature og trykk, men er linearisert med hensyn på sammensetning. D-spice var utvilsomt bedre tilpasset til det virkelige anlegget. Imidlertid, ble noe av dynamikken funnet å være mer troverdig i Unisim snarere enn i D-Spice. Problemet som ble funnet med Unisim var enkelhet i kolonnestruktur, hvor mer kompliserte strukturer resulterte med konvergensproblemer av løsningsmetodene.

Senere i denne studien, ble oppførsel til kontrollstrukturen undersøkt ved lavere føderate. Temperaturregulatorer var da i prioritet. Det ble funnet at en rett operasjon, som også ble funnet å være mest lønnsom, vil ikke resultere i kritisk ustabil prosess. Selv om det samme ikke kan sies om den ulønnsomme operasjon, ble gain scheduling funnet å være unødvendig verktøy hvis prosessen drives på en lønnsom måte og SIMC tuningsregler ligger i grunn.

Til slutt, ble det gjort optimalisering med minimering av kostnadsfunksjonen til den største destillasjonskolonnen. Optimaliseringen ble gjennomført med hensyn til urenheter av den lette komponenten i bunnproduktet, mens tungkomponent i toppen ble holdt konstant først på setpunktet til overordnede kontroll lag (Septic) og deretter på spesifikasjon av strømmen. Resultatet ble noe lavere urenheter av den lette komponenten i bunn enn den oppgitte spesifikasjonen. Kostnadsfunksjonen ble redusert med 1.6% fra spesifikasjonen til optimum verdi. Følgelig, ble real time optimization (RTO) anbefalt.

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Chapter 1

Introduction

There are different methods that are used to separate two or more components from each other. The one that is used widely in industry is called distillation which is based on differences in volatilities of the components. A standard distillation column has three functional units; cooler, condenser and reboiler. These units give several degrees of freedom that is used to define control structure of the column.

The feed that is entering the column can generally be classified by several variables, like for instance, feed rate, composition pressure and temperature. Together with product composition, these values contribute to the definition of the operation condition that column is currently operated on. Different control structures are used to stabilize and operate the column. In a real process plant the operation conditions may have large variance putting the controllers to test continuously. A big deviation from normal operation condition, the one controller was originally designed for, may result in totally different behavior at other operation conditions. An example of this is often seen when controllers that are tuned "tight" on high feed rate are used at much lower feed rates. The observations in such cases are too aggressive control and even undesired oscillations, making the term "stabilizing control" inappropriate.

Such aggressive behavior is sometimes observed in distillation train with three distillation column in series, at Kårstø, one of the Statoils gas processing plants. One of the motivations of this project is to find a reason for such behavior and propose a solution to the problem. For illustration of the problem and propose a solution how the unstable performance can prevented, it will be used two simulation programs, Unsim and D-spice. The

former are used by Statoil as simulation tool. The latter is simulation program widely used in researches at Norwegian University of Science and Technology (NTNU). The biggest distinction between the programs are calculation procedure. To make the calculations faster and more robust numerically, D-spice take advantages of thermodynamical tables, where thermodynamic properties are given for various temperature and pressure and linearized with respect to composition. Both of the programs will be used with a similar control structure as in the real plant with essential emphasis on a temperature controller, where control difficulties are observed.

Regarding tuning of the controllers, Sigurd Skogestad has introduced several tuning method for smooth tuning of the controllers making the controllers less sensitive to changes in operation condition (Skogestad & Grimholt 2011). Another alternative for avoiding the unwanted aggressive behavior of the controller is to consider adaptive control in the name of gain scheduling (Jang, Annaswamy & Lavretsky 2008). However, gain scheduling requires good understanding of how operation condition, including other variables like pressure, temperature, composition etc., influence the operation of a particular column. The use of gain scheduling of full extent could therefore be unnecessary complicated. In this study it will be investigated whether gain scheduling is generally required or not.

Another motivation of the thesis is consider current operation of the columns. Optimization, with respect to cost function of the most energy consumption column will be done. A benefit operation will be proposed. Elaboration of why moderate use of reboiler duty will not result in more benefit operation will be executed.

To summarize, this study will first compare the dynamics in the two simulation programs and investigate which of these resembles most to the performance in the real plant. Further, the study will find a reason of unstable behavior of temperature controller at low feed rate. Eventually, the final goal is to find whether it is possible to find more benefit operation of the distillation train, than it is presently operated, both at full feed rate and half feed rate.

Chapter 2

Theoretical background

2.1 Degrees of freedom

A systematic illustration of a distillation column is presented in figure 2.1. The illustration is a simplified model of all of the three columns that is used in a real process plant, with similar control structure. The feed in the process is given, the cooler is used to control the pressure and product streams are used as level controllers, The remaining degrees of freedom (DOF) are reboiler duty and reflux ratio. The latter is often set to control the reflux flow (FC), while temperature controller (TC) is often located at the lower part of the column as shown in figure 2.1.

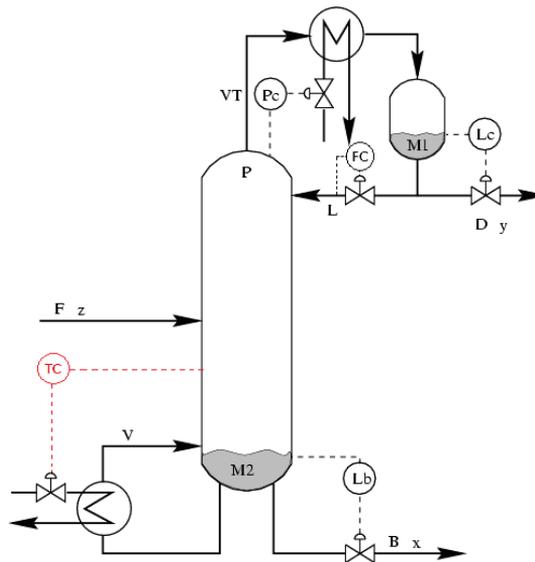


Figure 2.1: Systematic illustration of a simple distillation column, supplemented with a TC and FC. (Jacobsen & Skogestad 1993)

2.2 Temperature controller

The purpose of a temperature controller is to hold the temperature constant in one specific tray in a column. This can be done with either reflux or reboiler as manipulated variables, controlling the upper and lower part of the column respectively. A good choice of the tray provides more stable operation with disturbance in the feed. Furthermore, resulting in more or less stable production of the bottom and the top products of the column. Sigurd Skogestad has proposed interesting principles of how TC should be selected (Skogestad 2007) (Hori & Skogestad 2007). One of these papers (Hori & Skogestad 2007) presents examples of structures that are "reasonable" for different type of columns. The paper considers three types of disturbances: feed rate ($\Delta F = \pm 20\%$), feed composition ($\Delta z_F = \pm 10\%$) and fraction of liquid in the feed ($\Delta q_F = \pm 10\%$). However, both Skogestad and Luyben (Luyben 2005) point out that the main disturbances that should be taken into consideration are disturbances in the feed composition.

In addition, to find the best location of stabilizing temperature controller for all of three

types of disturbance, Skogestad and Hori (Hori & Skogestad 2007) propose some rules for finding best location of temperature controller:

1. Steepest slope in temperature profile
2. Small optimal variation with respect to disturbances
3. Large sensitivity to input change

Both the first and the last rule give the same result and usually favor locations away from the column ends, where the temperature slope is largest, while the second rule favors location close to the column ends. Methods like "max gain rule" and "exact local method" (Halvorsen, Skogestad, Morud & Alstad 2003) can give the best location of TC. However, the locations of the temperature controllers are established during the developing phase of the process plant and under no circumstances can be changed at this point. The idea is rather to investigate if the undesired control behavior can be explained by the fact that operation of the process is far from original design. A simple review of temperature profile could contribute to this study.

2.3 Fluid dynamics

Several changes in dynamics behavior can be observed when a column is operated with different feed rates than it was originally designed for. The most important changes that also influence the tuning of the controller are:

- Composition differences between two neighbor trays ($x_{i+1} - x_i$).
- Tray holdup (M_i).
- Time delay (Θ).

The first two subdivisions have direct effect on process gain and will be elucidated in subsection 2.3.1. The later will be more closely elaborated in subsection 2.3.2.

2.3.1 Process gain

Total material balance (equation 2.1) on stage "i" can be expressed with vapor flow up the column (V) and liquid flow down the column (L), as given in equation 2.2

$$\frac{d}{dt}(\text{Accumulated}) = In - Out \quad (2.1)$$

$$\frac{dM_i}{dt} = L_{i+1} - L_i + V_{i-1} - V_i \quad (2.2)$$

Taking into consideration component balance, results in equation 2.3

$$\frac{d(M_i x_i)}{dt} = L_{i+1} x_{i+1} - L_i x_i + V_{i-1} y_{i-1} - V_i y_i \quad (2.3)$$

With small change in fluid flow (ΔL), the vapor flow initially doesn't change. With some deduction, the equation above can be simplified as shown in equation 2.4.

$$\frac{d(M_i x_i)}{dt} = \Delta L(x_{i+1} - x_i) \quad (2.4)$$

Holdup can then be considered to be time invariant. The result is shown in equation 2.5.

$$\frac{dx}{dt} = \frac{\Delta L(x_{i+1} - x_i)}{M_i} \quad (2.5)$$

The equation above can be transformed to show the temperature changes as function of time by making assumption that temperature is only dependent on fluid composition at each stage (2.6). The deduction is given in equations 2.7-2.8 and result is shown in equation 2.9.

$$T_i = x_i T_{b1} + (1 - x_i) T_{b2} \quad (2.6)$$

$$x_i = \frac{T_i - T_{b2}}{T_{b1} - T_{b2}} \quad (2.7)$$

Equation above is then differentiated and inserted in equation 2.5.

$$\frac{1}{T_{b1} - T_{b2}} \frac{dT_i}{dt} = \frac{\Delta L \left(\frac{T_{i+1} - T_{b2}}{T_{b1} - T_{b2}} - \frac{T_i - T_{b2}}{T_{b1} - T_{b2}} \right)}{M_i} \quad (2.8)$$

$$\frac{dT_i}{dt} = \frac{\Delta L(T_{i+1} - T_i)}{M_i} \quad (2.9)$$

Process gain (k') can then be expressed as the change in temperature at the tray divided by the change in fluid flow. The results will then be that fluid dynamic at one specific tray is only dependent on difference in the temperature on the tray above and on the tray itself and holdup at the tray, as shown in equation 2.10. The same equation will also be valid in cases with more than two components in the fluid.

$$k' = \frac{1}{\Delta L} \frac{dT_i}{dt} = \frac{T_{i+1} - T_i}{M_i} \quad (2.10)$$

Both temperature difference and tray holdup are stationary values. The former is determined by such factors as composition in the feed and product streams and can be ascertained by the temperature profile of the column. The determination of temperature profile, and therefore temperature differences, can be done by handful temperature measurements scattered over the column, while tray holdup is more complex to assign.

Tray holdup

Per definition, tray holdup can be divided into liquid on the sieve tray and downcomer (Wittgens & Skogestad 2000) and therefore hard dependent on the flow of the fluid in the column (L). The correlation between M and L can be described by simplified Francis weir formula (Skogestad & Morari 1988):

$$M_{0i} = k_1 L_i^{2/3} \quad (2.11)$$

Making the assumption that holdup is the same at each tray and $k_1 = k_2 = k_i$, the ratio of two independent operation points yields:

$$\frac{M_0}{M_1} = \frac{k_1}{k_2} \left(\frac{L_0}{L_1}\right)^{2/3} = \left(\frac{L_0}{L_1}\right)^{2/3} \quad (2.12)$$

Rearranging equation 2.12 and making another approximation that reflux (L) and reboiler duty (V) are equally depended on feed rate (F), yields in equation 2.13:

$$M_1 = M_0 \left(\frac{V_1}{V_0} \right)^{2/3} \quad (2.13)$$

In the article "Evaluation of Dynamic Models of Distillation Columns with Emphasis on the Initial Response" (Wittgens & Skogestad 2000) Bernd Wittgens and Sigurd Skogestad looked at tray holdup in more detail. The idea is to split the holdup in several sections where liquid can be found, i.e. sieve tray, downcomer, inlet and outlet weir. As in the previous deduction, the basis of varying height over weir was taken in Francis weir formula, but in this case the formula was modified. The result is presented in equation 2.14.

$$h_{ow} = 44300 \cdot \left(\frac{L_{out}}{\rho_l \cdot 0.5 \cdot d_{weir}} \right)^{0.704} \quad (2.14)$$

However, taking a ratio between two independent operation points of the columns yields the same equation 2.13 with exponential factor 0.704 instead of 2/3.

2.3.2 Delay in the reboiler

The saturated steam that is entering the reboiler goes through several time consuming stages. First of all, steam condenses in the shell side of the reboiler, then the heat is transferred through the wall, and eventually the fluid in the tube side of the reboiler is warmed up. Numerous bubbles that are formed generas the driving force in the column. The described dynamics are often neglected. The reason for that is that the time scale is often much smaller compared to other dynamics in the column. Instead delay (Θ), given by equation 2.15, with varying value at different operation point, is often included.

$$\Theta = \frac{M_0}{L} \approx L^{-1} \quad (2.15)$$

Approximation is made based on the fact that holdup is constant in condenser (M_D) and reboiler (M_B). The approximation that L and V are equally depended on F that was made in subsection 2.3.1 can also be made here, resulting in equation 2.16:

$$\Theta_1 = \Theta_0 \cdot \frac{V_0}{V_1} \quad (2.16)$$

Where V_0 and Θ_0 are initial reboiler duty and corresponding delay, respectively.

2.4 Tuning of the temperature controller

The SIMC tuning rules (Skogestad & Grimholt 2011) are some of the useful rules to implement on PID controllers. In this report, the rules were therefore implemented to tune the temperature controller. Generally, tuning rules can be described as presented in equation 2.17-2.18, with controller gain (K_c) and time constant (τ_I) as tuning parameters:

$$K_c = \frac{1}{k} \cdot \frac{\tau_1}{\tau_c + \Theta} = \frac{1}{k'} \cdot \frac{1}{\tau_c + \Theta} \quad (2.17)$$

$$\tau_I = \min \{4(\tau_c + \Theta), \tau_1\} \quad (2.18)$$

Where $k = \Delta y / \Delta u$ and τ_c , the desired first-order closed-loop time constant τ_c , is the only tuning parameter. Further, two assumption can be made; that $\tau_c = c \cdot \Theta$ with $c \geq 1$ and $\tau_c + \Theta \ll \tau_1$. This results that equations 2.17 and 2.18 gives equations 2.19 and 2.20 respectively.

$$K_c = \frac{1}{k' \cdot \Theta} \cdot \frac{1}{(c + 1)} \quad (2.19)$$

$$\tau_I = 4\Theta \cdot (c + 1) \quad (2.20)$$

Equation 2.19 shows that when c is a constant the factor $k' \cdot \Theta$ is one and only that decides K_c . While in equation 2.20 it is pure delay that decides the time constant for the controller.

2.5 Minimization of the costs

The cost to be minimized in a distillation column, from the economic point of view, can generally be expressed with equation 2.21, where first two terms express cost of feed and energy (heating and cooling) respectively and the last two terms are the value products.

$$J = -P = p_F F + p_V V - p_D D - p_B B \quad (2.21)$$

Further, the cost function can be divided by price of the feed (p_f), to give:

$$\frac{J}{p_f} = F + \frac{p_V}{p_f}V - \frac{p_D}{p_f}D - \frac{p_B}{p_f}B \quad (2.22)$$

or,

$$J' = F + p'_V V - p'_D D - p'_B B \quad (2.23)$$

In the case where sea water is used as cooling medium in Butane Splitter, the cost of cooling in condensers can be neglected. The second term can then be expressed as ratio between evaporation enthalpy ($\Delta_{vap}H$) and combustion enthalpy ($\Delta_c H$) multiplied with vapor flow (V), by the simple assumption that gas in the column is the same that is used as combustion gas. Where combustion gas includes often only light or medium light components. The ratio of $\frac{\Delta_{vap}H}{\Delta_c H}$ has a value of 0.00982 for ethane and 0.00856 for propane. For simplicity the values was set to be 0.01 . The equation above can then be expressed as shown in equation 2.24

$$J' = F + 0.01V_{vap} - p'_D D - p'_B B \quad (2.24)$$

Further derivation and implementation of the equation above is given in subsection 3.4.

Chapter 3

Modeling and implementation

Two simulation programs were used in this study with different calculation approach. D-spice is the program that is used as simulation program at Kårstø for the entire process plant, and naturally also the train 24, with three distillation columns in series. The simulation program is a convenient tool that covers the whole plant in very practical way. The second program that is used in this report as simulation program for comparison, is Unisim. The program is frequently used as simulation tool at NTNU and has also many advantages. However, one of the biggest distinctions between Unisim and D-spice is that D-spice takes advantages of thermodynamical tables, where thermodynamic properties are given for various temperatures and pressures and linearized with respect to compositions. While Unisim utilize the numerous thermodynamical equations. This way Unisim can be slower, but more accurate and smooth in its calculations than D-spice.

Initially in this study there were made stationary models of the distillation columns in Unisim. Subsequently, these models were converted to dynamics models for dynamic simulation and comparison with D-spice. The highlights during the development are presented stepwise in subsection 3.1. The utilized models in D-spice are, per definition, outdated, but are very similar to the models used in the plant. During the fitting of Unisim to the real plant, some of parameters in D-spice were therefore imported.

3.1 Model development in Unisim

Originally, the steady state model of the process was made. Further, sizing of the equipments and pressure flow specification, including installation of required valves, was done. The process flow diagram of the model is presented in figure 3.1. The biggest discrepancy between the real plant and Unisim is that, due to some package problems, could not split cooler and condenser in two separate units. The main effect is slightly different control structure. This is elaborated in section 3.2.

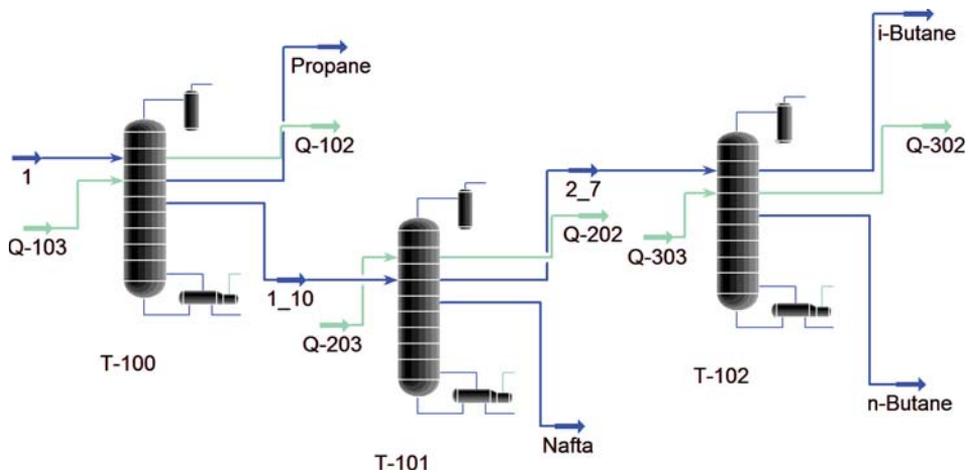


Figure 3.1: Process flow diagram of three columns in a row, with Depropaniser, Debutaniser and Butane Splitter set up subsequently. "Nafta" stream is referred to "Naphtha", bottom stream leaving the Depropaniser.

3.1.1 Dimensioning of the equipment

Numerous dimensioning and rating data was adapted from D-spice. This includes such factors as number of stages, tray space, weir height, weir length and diameter of the columns, but also length and diameter of condensers and reboilers.

3.1.2 Pressure drop over the columns

Average pressure drops over the columns in the real plant, during a timescale of a month, are presented in table 3.1. Generally, pressure drop can be determined by the static head

(wet), that is caused by the liquid on the trays and the frictional (dry) pressure drop through the holes of the tray. This is shown in equation 3.1.

$$\Delta p = \Delta p_{static} + \Delta p_{dry} \quad (3.1)$$

Static head pressure drop is determined by factors like weir height and weir length which was set during the dimensioning of the columns. For the best reproduction of the plant to the models in Unisim, k-factor was used to achieve the right pressure drops over the columns.

Table 3.1: Pressure drops over the columns at full feed rate.

Column	Pressure drop [mbar]	
	Unisim	D-spice
Depropaniser	310	348
Debutaniser	260	636
Butansplitter	824	862

3.1.3 K-factor

Unisim uses k-factor to determine flow between stages. The default calculation used by Unisim is based on the column diameter (equation 3.2).

$$k \propto (d)^2 \quad (3.2)$$

Where d is a diameter of the specific tray in the column.

This simplification of k-factor serves good when some remaining parts of the column is applied default dimension. In cases when transition between the steady state and dynamic simulation resulted in resetting dimension of some part the process in a wrong way, a correction of the k-factor, presented in equation 3.3, was necessary.

$$k = \frac{\dot{m}}{\sqrt{\rho_v \cdot \Delta p_f}} \quad (3.3)$$

Where, \dot{m} [kg/h] is vapor flow, ρ [kg/m³] is density of vapor and p_f [kPa] is friction pressure losses. Regarding the latter, this one can be derived regarding pressure difference between two adjacent stages.

$$\Delta p = p_i - p_{i-1} \quad (3.4)$$

Further deduction of equation 3.1 is shown in equation 3.5.

$$\Delta p = \Delta p_{static} + \Delta p_{dry} = \rho_l g h + \left(\frac{\dot{m}}{k}\right)^2 \frac{1}{\rho_v} \quad (3.5)$$

Where ρ is density and h is height of the liquid in the tray and Δp_{dry} is obtained from equation 3.3. The first term in the equation above is determined by Unisim, where weir height and length is used in the calculations. This static head pressure drop and the desired pressure drop between two adjacent stages, which was set to be the total pressure drop over the column divided by the number of stages, was used to calculate k-factor:

$$k = \frac{\dot{m}}{((\Delta p - \Delta p_{static})\rho_v)^{1/2}} \quad (3.6)$$

In the calculation Unisim takes into consideration more factors then presented here, and final marginal adjustment of the k-factor was therefore done manually to obtain the right pressure drop over the column. The same procedure was applied in all of the three columns.

3.1.4 Adaption of the dynamics

The dynamics in the columns can generally be described by process gain (k') and time delay (Θ). These values, regarding Butane Splitter, are presented in table 3.2, which are obtained from the analysis of step response in the temperature controller with step in the output. (Appendix A). In Unisim, delay was fitted to the plant value through a regression to obtain the similar response. This was done by implementation of transfer function, as shown in figure 3.2.

Table 3.2: Process gain and time delay in the TC in Butane Splitter.

	k'	Θ [min]
91% feed rate (<i>Plant</i>) ¹⁾	0.0421	2.00
66% feed rate (<i>Plant</i>)	0.0267	2.43
100% feed rate (<i>Unisim</i>) ²⁾	0.0237	2.00
100% feed rate (<i>D – Spice</i>)	0.0989	0.17

1) Different composition in the feed. 2) Fitted with data obtained from the plant.

3.2 Controller structure

The setup of the controllers was identical in all three columns in Unisim. A figure illustrating location of all of the controllers in the Depropaniser is shown in figure 3.2. The description and location of the controllers is given in table 3.3. The tuning of controllers were done by the SIMC method (Skogestad & Grimholt 2011).

Table 3.3: Controllers present in the model developed in Unisim. Where "X" represents 1(Propaniser), 2(Debutaniser) and 3(Butane Splitter), with temperature controller location (Y) at stage 11, 6 and 7, respectively.

Controller	Description	Location
FIC-X00	Flow controller	Reflux stream
PIC-X01	Pressure controller	Condenser (Unisim) or stream entering the condenser (D-spice)
LIC-X02	Level controller	Condenser
LIC-X03	Level controller	Reboiler
TIC-X04	Temperature controller	Stage Y

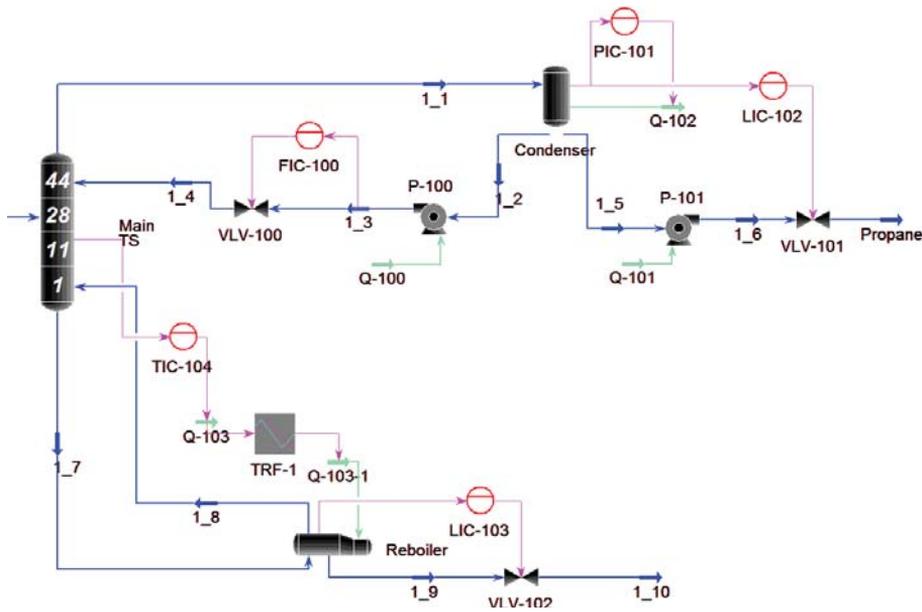


Figure 3.2: Process flow diagram with controllers structure in the Depropaniser.

The biggest distinction between the control structure in Unisim and the plant is located in the cooler. The problem with splitting the cooler and condenser in two separate units resulted in different control structure. The absence of bypass through the cooler before the entrance in condenser, made it necessary to implement pressure controller directly in duty of condenser, as shown in figure 3.2. This resulted in slightly slower response and somewhat ductile pressure control.

3.3 Operation points

The objectives for the project was to compare dynamics in Unisim with dynamics in D-spice and then observe how they changes with different feed rates. Whereupon observe how temperature controller, but also other controllers behaves at these conditions. Based on these condition there were defined 3 operation points. The first operation point is defined as a point of reference, corresponding to full operation at full feed rate. The letter two operation points are defined at half feed rate, but with different assigned priorities in composition of product streams. All three operation points, for all three columns are presented in table 3.4, with Depropaniser, Debutaniser and Butane Splitter defined as column

1-3, respectively. Closer elaboration of operation points are presented in subsections 3.3.1-3.3.3.

Table 3.4: Definition of different operation points. Specified values are marked bold.

Operation point	Column	F [kg/h]	L [kg/h]	V [kg/h]	$x_{D,i}$ [%]	$x_{B,i}$ [%]	T [°C]
	1	2.430E5	1.908E5	3.291E5	0.95 (ic4)	0.20 ¹⁾ (c3)	80.82
1	2	1.103E5	7.648E4	1.083E5	0.52 ²⁾ (c5+)	1.0 (nc4)	81.56
	3	6.573E4	2.247E5	2.397E5	2.00 (nc4)	1.25 (ic4)	52.68
	1	1.215E5	1.431E5	2.156E5	0.08 (ic4)	0.20 ¹⁾ (c3)	75.81
2	2	5.602E4	5.720E4	7.501E4	0.50 ²⁾ (c5+)	0.02 (nc4)	89.53
	3	3.388E4	1.675E5	1.730E5	2.00 (nc4)	0.08 (ic4)	52.21
	1	1.215E5	1.431E5	2.156E5	0.08 (ic4)	0.20 (c3)	75.81
3	2	5.602E4	5.720e4	7.388E4	0.01 (c5+)	1.00 (nc4)	78.23
	3	3.351E4	1.675E5	1.724E5	0.12 (nc4)	1.25 (ic4)	51.61

1) Actual specification correspond to 0.85% c3 in top stream of Butane Splitter

2) Actual specification correspond to 0.8% c5+ in bottom stream of Butane Splitter

Temperature profiles for all of these columns are presented in figures 3.3- 3.5.

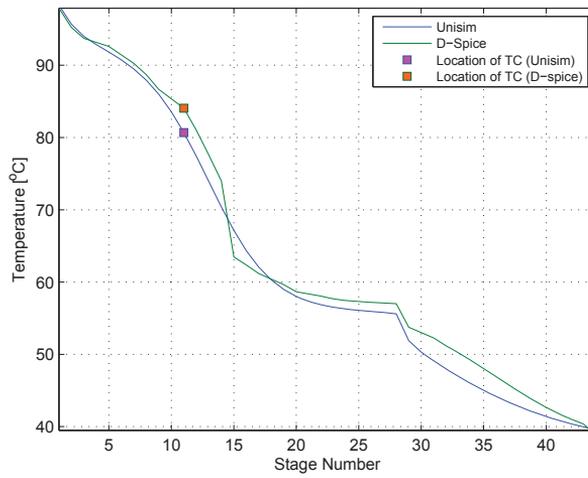


Figure 3.3: Temperature profile of Depropaniser in both Unisim and D-spice, at the same operation conditions.

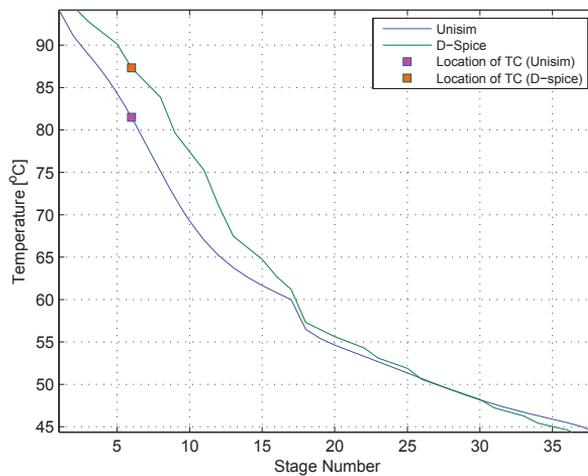


Figure 3.4: Temperature profile of Debutaniser in both Unisim and D-spice, at the same operation conditions.

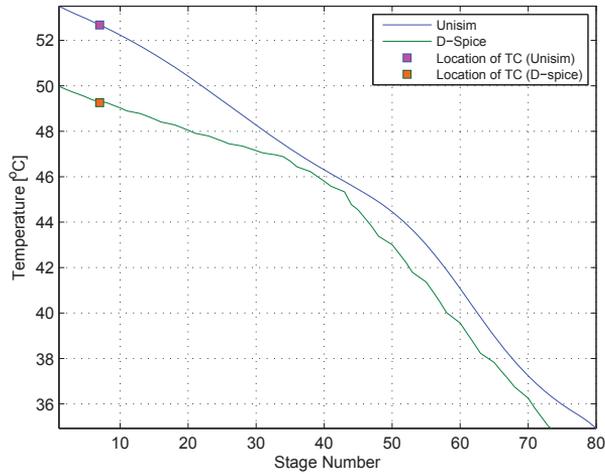


Figure 3.5: Temperature profile of Butane splitter in both Unisim and D-spice, at the same operation conditions.

3.3.1 Operation point 1, full rate

The first operation point was made as a point of reference, corresponding to full operation at full feed rate. All of the variables defining the feed stream were exported from D-spice. In the process plant a supervisory control layer, Septic is always active at full feed rate, with back off from constrain with 50%. Specifications in composition of the product streams were therefore adopted from Septic.

3.3.2 Operation point 2, half rate, profitable operation

Operation point 2 were identified to be at exactly 50% feed rate from the complete feed rate operation. All of the other feed variables like for instance, pressure, temperature and composition is kept unchanged from operation point 1. In spite of ideology that both reboiler duty and reflux rate is linear dependent on feed rate, this statement will not hold in practice. The reason for that is that such low reflux rate would probably result in weeping in the column, due to low vapor flow in the column. For that reason, the reflux constraints for all of the column was defined to be 75% of the steady state value at full feed rate. The result is a loss of the manipulated variable.

Further, it was necessary to define which product stream composition should be remained

as control variable and which should be ignored and therefore overpurified. Operation point 2 was defined in such way that most of valuable i-butane should be kept inside the system before distillate in the last column where it is sold with half of impurity constraint. Stated differently, supervisory control layer, Septic, is operated on setpoint in bottom product composition in Propaniser and distillate composition in Depropaniser and Butane Splitter. All of the other impurity measurement are ignored.

3.3.3 Operation point 3, half rate, non profitable operation

Similar to operation point 2, constraint on reflux becomes active at half feed rate in all of the columns. Therefore definition of which product stream composition should be remained as control variable and which should be ignored and therefore over purified, is unavoidable. Despite of the fact that Depropaniser was held unchanged from the previous operation point, operation point 3 was defined in a contrary way. In this case, most of valuable i-butane is released through streams like Naphtha and n-Butane (figure 3.1). Unfortunately, in practice, this operation is more frequently preferred, rather than the profitable operation 2.

3.4 Optimization at full rate operation

Specifications of the product streams in the last two columns are presented in table 3.5, with names of the product streams presented in figure 3.1. All of the specifications, except from the specifications in product stream "Naphtha" are stated in mole per cent. The exceptional specification is done in respect to Reid Vapor Pressure (RVP).

The RVP measurement is done by the test method ASTM-D-323 for evaluation of volatility of the gasoline. In this case the method is applied to volatile nonviscous petroleum liquids, light Naphtha containing mostly i-heptane, n-heptane and n-hexane, but also traces of components up to n-decane. RVP is determine the absolute vapor pressure exerted by volatile liquid at $37.8^{\circ}C$ ($100^{\circ}F$). At the defined condition in the stream Naphtha, 2.0% of n-butane correspond to RVP value of 0.89 bar, while 1.0% of n-butane in the same stream correspond to RVP value of 0.87 bar.

Some of the product streams are subsequently mixed with other products, while some of them are sold as pure products. The prices, at which products are sold for, are kept within companies walls and are not taken into consideration in this study. However, there are two

possible alternatives. The first one takes into consideration that the prices of the product streams are the same. The most profitable operation, in such case, would be with product streams on the specifications, minimizing the reboiler duty. These specifications of the product streams from the last two columns are presented in table 3.5.

Table 3.5: Specifications of product streams.

Product stream	Low purity constraint on weight per cent basis [wt%]	High constraint on bi-components
I-butane	95	1.3% C3, 4% nC4
N-butane	95	1.5% C3, 2.5% iC4, 2.0% C5+
Naphtha	95	RVP=0.89 bar (2.0% nC4)

The second alternative regards the fact that i-butane is more demanded component than n-butane and naphtha due to several cases, like for instance high octane number. The price of the demanded component could therefore be set to be a fraction higher than for n-butane. In this case, the most profitable operation is doubtful with distillate on the specification, in terms of selling price is often the same regardless of component mixture, as long as it is kept under the specifications. Regarding the bottom stream, an optimization is elaborated to find at which impurity fraction (i-butane in bottom product) the operation becomes optimum.

The case with different prices per ton of sold components is the most reasonable. However, since the prices are hold concealed, the ratio of market prices between i-butane and n-butane was by a conjecture set to be the value of 1.5. The optimization was done on the most energy demanding column, Butane Splitter with equation 3.7, that is the modified adaption of equation 2.24.

$$J' = J_{splitter} = F_{splitter} + 0.01V_{splitter} - 1.5D_{i-butane} - 1B_{n-butane} \quad (3.7)$$

Where $F_{splitter}$ and $V_{splitter}$ stand for feed flow [kg/h] and vapor flow [kg/h] in the Butane Splitter. The former is a constant term in the optimization. Comparison of J function value in optimal operation, regarding impurity fraction of light component in the bottom product ($x_{B,ic4}$), as well as function value with product streams kept at their specifications were made. Comparison of J function value with product streams on set point utilized by MPC were also evaluated. This is presented in section 4.3.

Chapter 4

Results

4.1 Tuning results

Tuning of all of the controllers was done by equations 2.17 and 2.18. Most of the controllers, both in Unisim and D-Spice was found to have integrating open loop step response, with $\tau_1 \gg 4(\tau_c + \Theta)$. The tuning results of these controllers are presented in appendix B. Exclusively two and three pressure controllers in D-Spice and Unisim, respectively, were found to have small enough τ_1 to be tuned with SIMC first order tuning rules. These tuning results are presented in table 4.1

Table 4.1: First order PI tuning results of the pressure controllers.

Controller	Process			Control		
	Θ	k	τ_1	τ_c	K_c	τ_I [min]
PIC-101 (Unisim)	0	0.9786	0.458	2.00	1.5854	0.46
PIC-201 (Unisim)	0	1.2667	1.390	2.00	0.5487	1.39
PIC-301 (Unisim)	0	0.4762	1.500	2.00	1.5750	1.50
24_PC4016 (D-Spice)	-	-	-	-	-	-
24_PC4072 (D-Spice)	0	0.7520	0.7167	0.5	1.9060	0.72
24_PC4136 (D-Spice)	0	0.3267	0.8167	0.5	5.0000	0.82

Ultimately, temperature controller was tuned at full feed rate and later at the remaining operation points. In all of the cases the tuning was done with the same equations 2.17 and 2.18, assuming pure integrating response. Tuning parameter, τ_c , was set to be $2.5 \cdot \Theta$

for all three temperature controllers in Unisim. In D-spice the same parameter was more adapted to the one used in real plant, since the model in the program should represent the real process considerable better then the model in Unisim. The results of the tuning are presented in tables 4.2 and 4.3.

Table 4.2: First order PI tuning results of the temperature controllers in Unisim.

Operation point	Controller	Process		Control			
		Θ	k'	τ_c	K_c	τ_I [min]	τ_I [s]
1	TIC-104	2.00	0.1699	5.00	0.8408	28	1680
	TIC-204	2.00	0.1725	5.00	0.8282	28	1680
	TIC-304	2.00	0.0237	5.00	6.0277	28	1680
2	TIC-104	3.05	0.3858	7.64	0.2425	30.54	1833
	TIC-204	2.89	0.0654	7.22	1.5125	28.87	1732
	TIC-304	2.51	0.0297	6.28	3.8321	35.19	2112
3	TIC-104	3.05	0.3858	7.63	0.2425	42.76	2565
	TIC-204	2.93	0.3067	7.33	0.3178	41.04	2463
	TIC-304	2.52	0.0512	6.30	2.2164	35.28	2117

Table 4.3: First order PI tuning results of the temperature controllers in D-Spice.

Operation point	Controller	Process		Control			
		Θ	k'	τ_c	K_c	τ_I [min]	τ_I [s]
1	24.TC4008	0.17	0.7054	2.50	0.5309	10.68	641
	24.TIC4062	0.20	0.2474	4.00	0.9624	16.80	1008
	24.TC4113	0.17	0.0989	4.00	2.4248	16.68	1001
2	24.TC4008	0.27	0.7683	2.50	0.4699	11.08	665
	24.TIC4062	0.12	0.1768	4.00	1.3728	16.48	989
	24.TC4113	0.12	0.0818	4.00	2.9672	16.48	989
3	24.TC4008	0.12	0.7683	2.50	0.4968	10.48	629
	24.TIC4062	0.20	0.5977	4.00	0.3984	16.80	1008
	24.TC4113	0.15	0.0867	4.00	2.7793	16.60	996

4.2 Simulation results

Performances of the temperature controllers and corresponding changes in product streams from Butane Splitter at operation point 1-3 are presented in subsections 4.2.1 - 4.2.3, respectively. In all of the simulation it was done one disturbance in the feed rate ($dF = 10\%$) after 0.5 hour and one in the feed composition ($dzF_{Propane} = 4\%$) after 7 hours. Complete simulation results, with performance of all of the controllers in Unisim and corresponding

controllers in D-Spice, are introduced in appendixes C- E.

Eventually, another simulation was performed, at nonprofitable operation point 3. This time simulation was done with retuned PI controller parameters retuned at current operation point. This way it was shown that the smooth tuning of other controllers didn't result in oscillatory behavior at different operation condition, what was the case with temperature controller. Stated differently, the oscillation observed at the same operation condition was caused by temperature controller only, and not the other controllers. The simulation can be found in appendix F.

4.2.1 Simulation at operation point 1

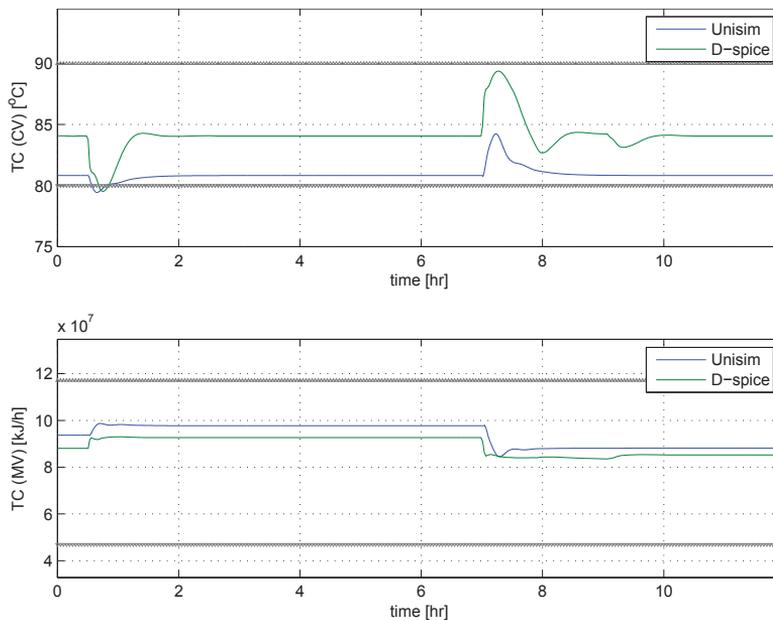


Figure 4.1: Behavior of manipulated and controlled variables for temperature controller in Depropaniser at full rate.

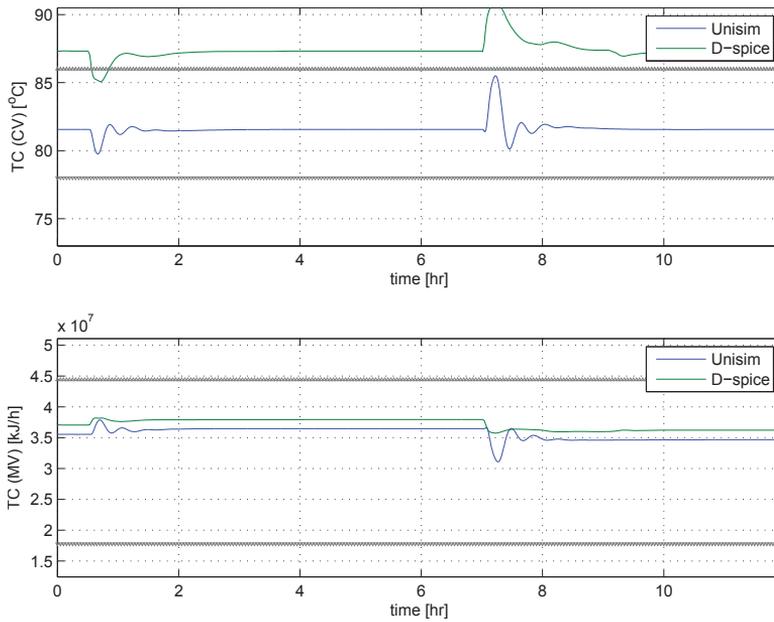


Figure 4.2: Behavior of manipulated and controlled variables for temperature controller in Debutaniser at full rate.

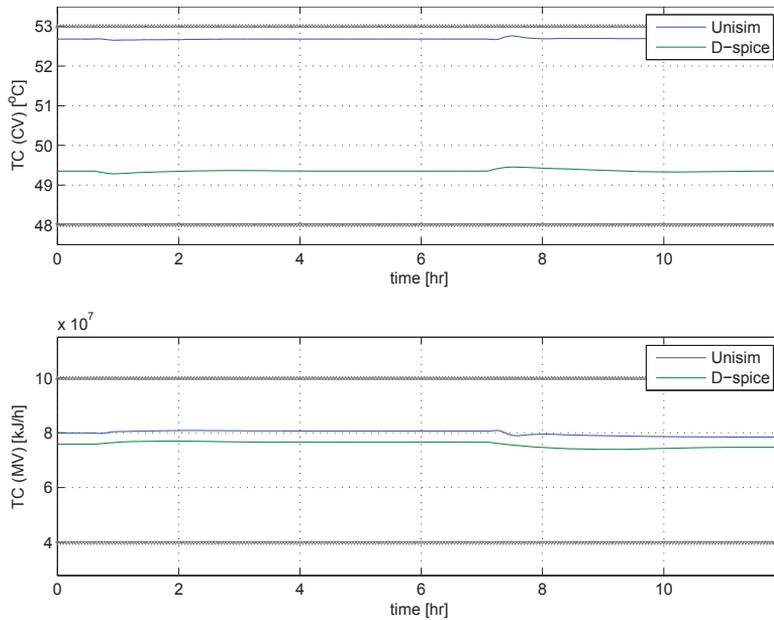


Figure 4.3: Behavior of manipulated and controlled variables for temperature controller in Butane Splitter at full rate.

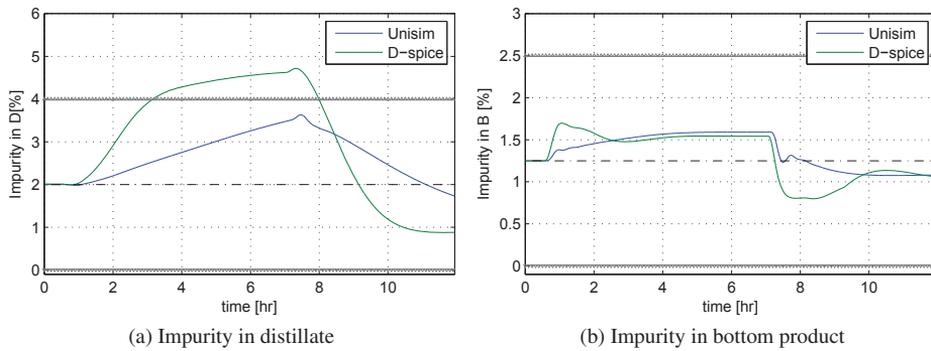


Figure 4.4: Impurities in distillate ($x_{D,c4}$) and bottom product ($x_{B,ic4}$) in the Butane Splitter at full rate.

4.2.2 Simulation at operation point 2

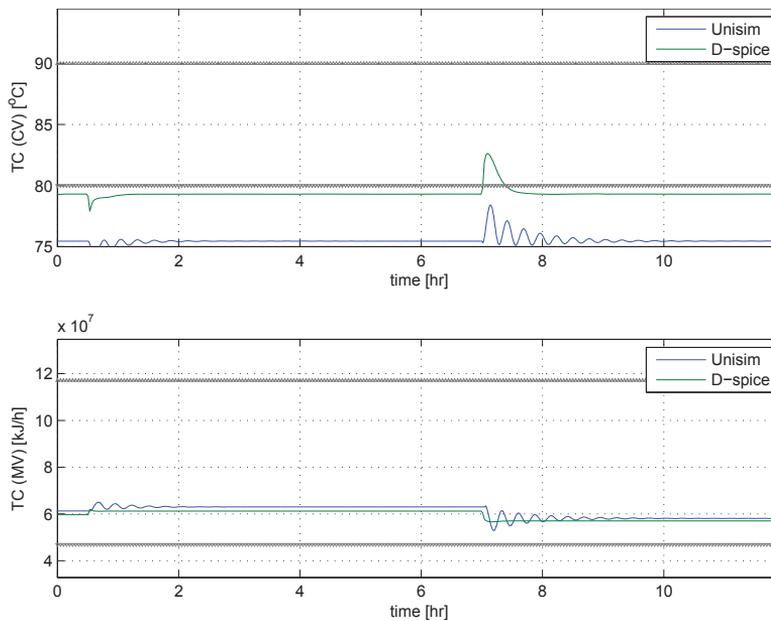


Figure 4.5: Behavior of manipulated and controlled variables for temperature controller in Depropaniser at profitable operation 3 with 50% feed rate..

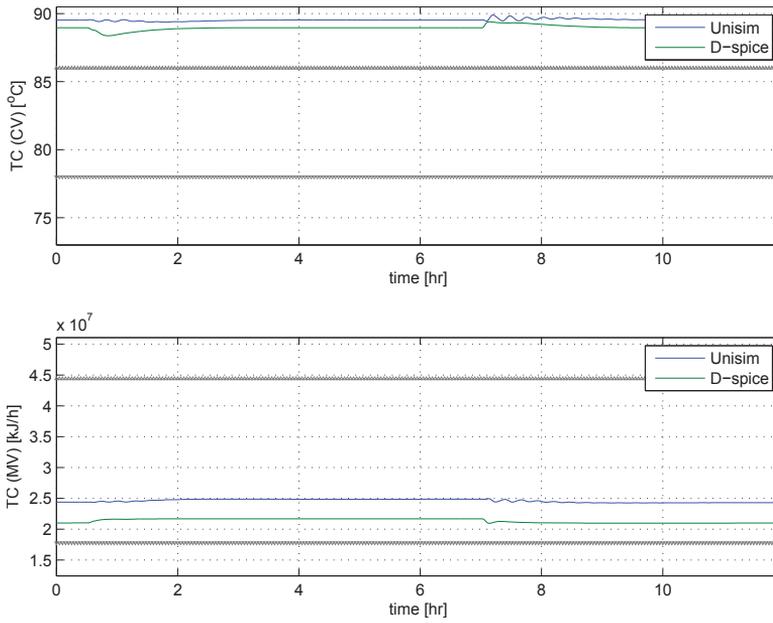


Figure 4.6: Behavior of manipulated and controlled variables for temperature controller in Debutaniser at profitable operation 3 with 50% feed rate..

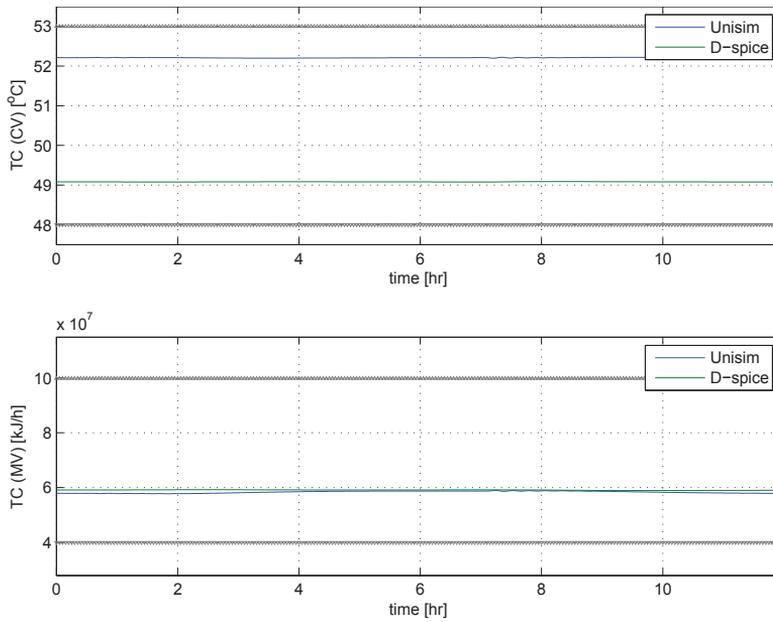


Figure 4.7: Behavior of manipulated and controlled variables for temperature controller in Butane Splitter at profitable operation 3 with 50% feed rate..

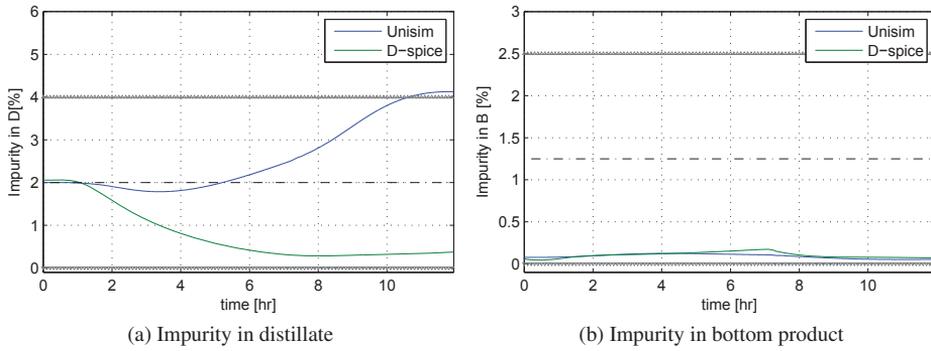


Figure 4.8: Impurities in distillate ($x_{D,c4}$) and bottom product ($x_{B,ic4}$) in the Butane Splitter at profitable operation 3 with 50% feed rate..

4.2.3 Simulation at operation point 3

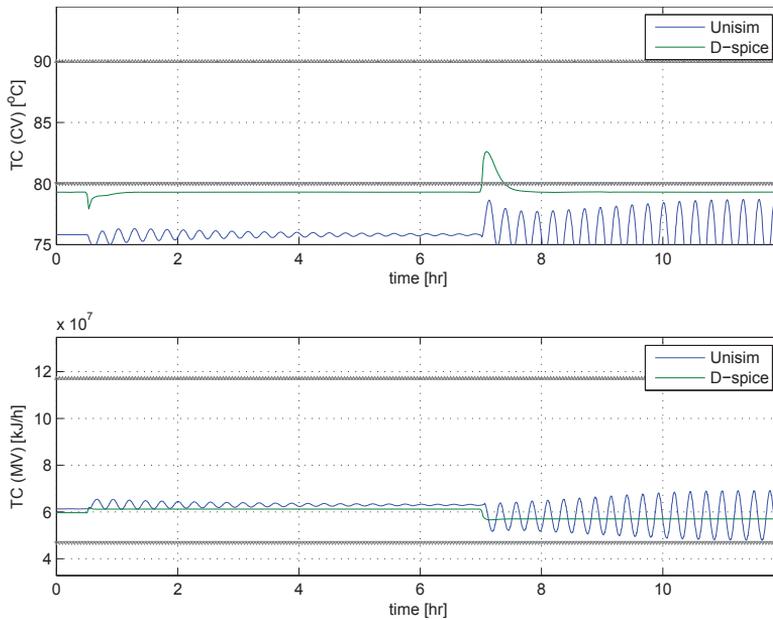


Figure 4.9: Behavior of manipulated and controlled variables for temperature controller in Depropaniser at nonprofitable operation 3 with 50% feed rate.

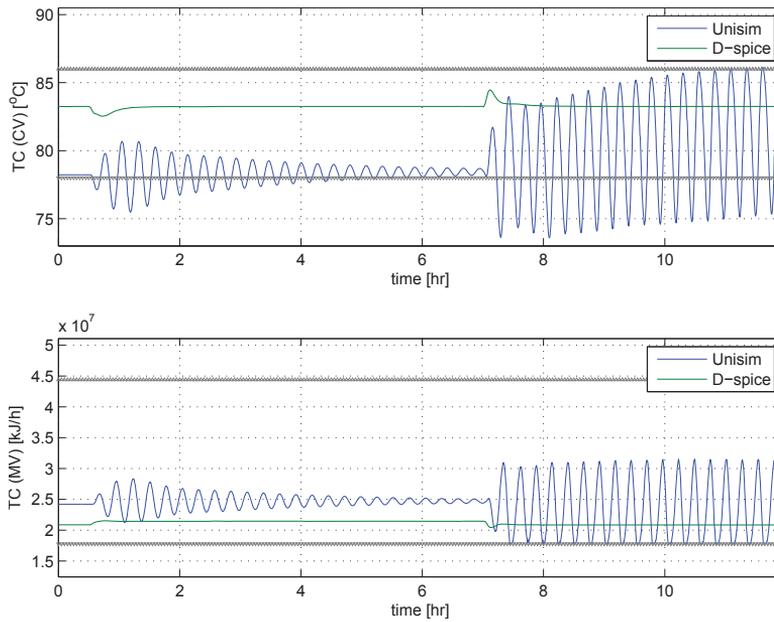


Figure 4.10: Behavior of manipulated and controlled variables for temperature controller in Debutaniser at non-profitable operation 3 with 50% feed rate.

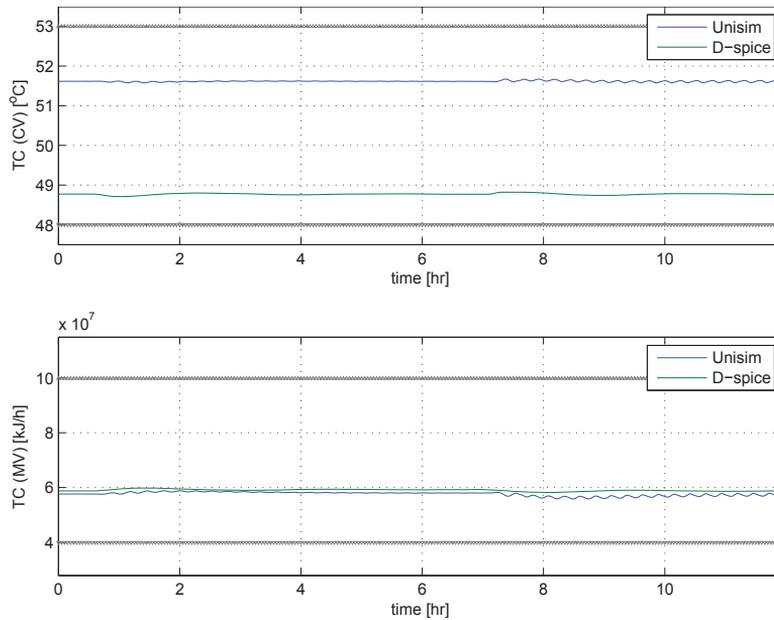


Figure 4.11: Behavior of manipulated and controlled variables for temperature controller in Butane Splitter at non-profitable operation 3 with 50% feed rate.

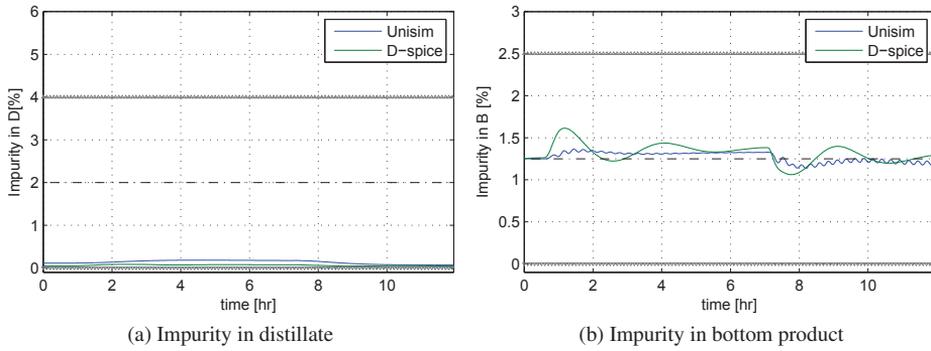


Figure 4.12: Impurities in distillate ($x_{D,c4}$) and bottom product ($x_{B,ic4}$) in the Butane Splitter at non-profitable operation 3 with 50% feed rate.

4.2.4 Simulation at operation point 3, with retuned TC

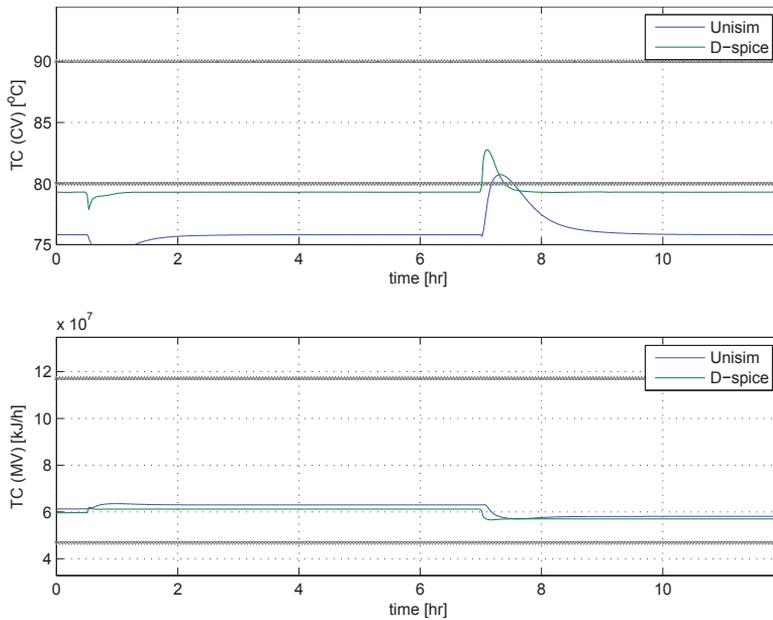


Figure 4.13: Behavior of manipulated and controlled variables for temperature controller (retuned) in Depropaniser at non-profitable operation 3 with 50% feed rate.

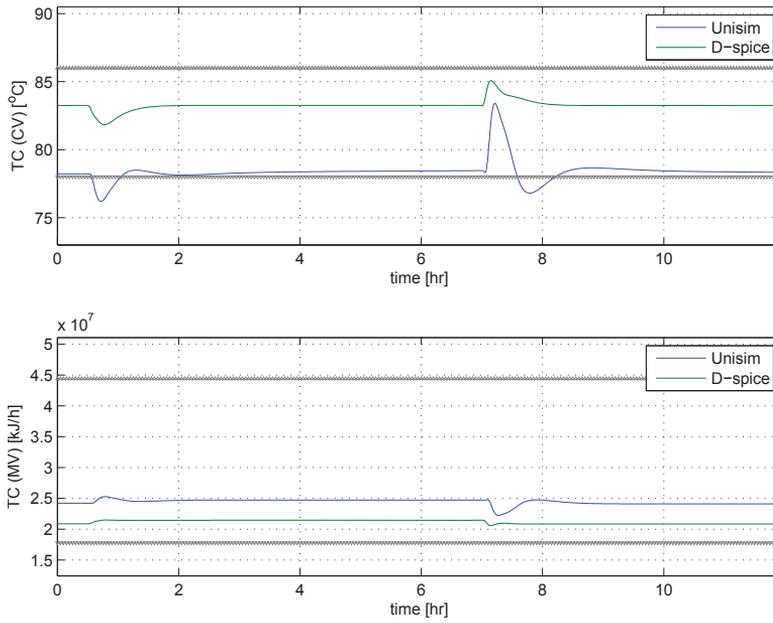


Figure 4.14: Behavior of manipulated and controlled variables for temperature controller (retuned) in Debutaniser at non-profitable operation 3 with 50% feed rate.

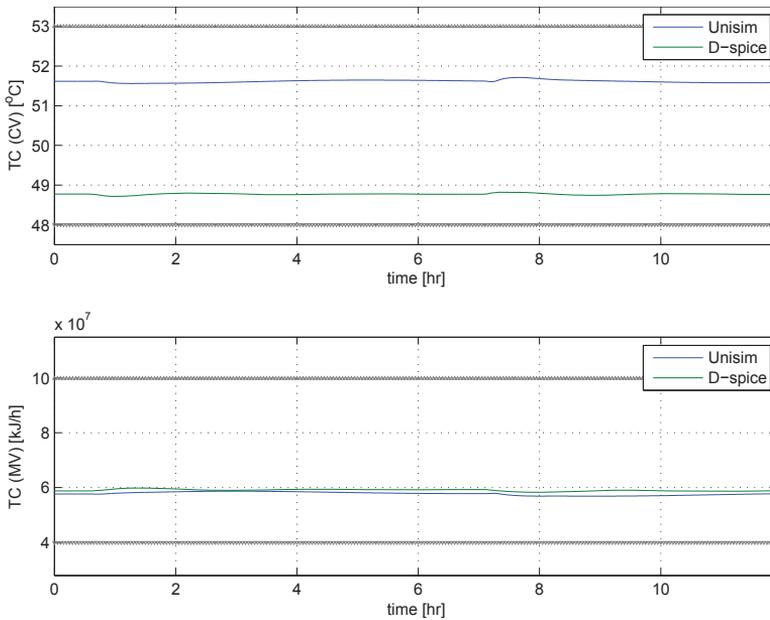


Figure 4.15: Behavior of manipulated and controlled variables for temperature controller (retuned) in Butane Splitter at non-profitable operation 3 with 50% feed rate.

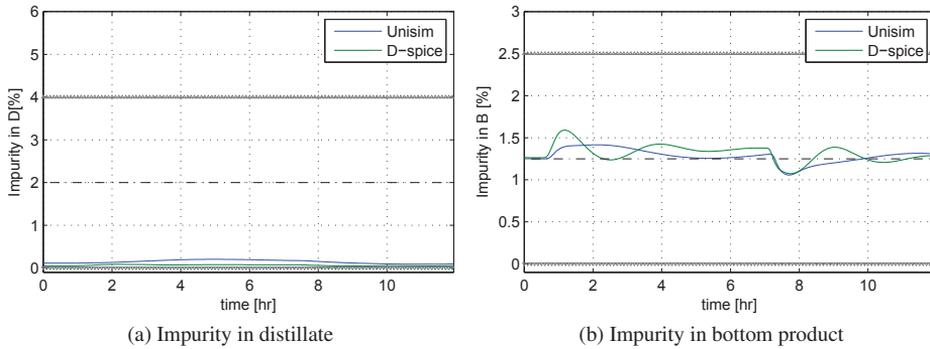


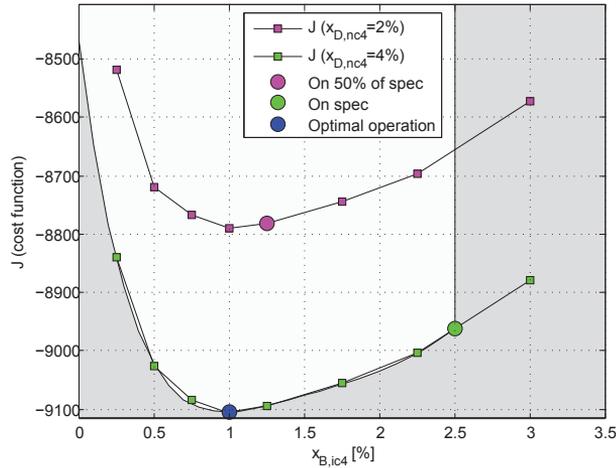
Figure 4.16: Impurities in distillate ($x_{D,c4}$) and bottom product ($x_{B,ic4}$) in the Butane Splitter at non-profitable operation 3 with 50% feed rate.

4.3 Optimization results

The optimization, regarding impurity fraction of light component in the bottom product ($x_{B,ic4}$) were done with two constant values of impurity fraction of heavy component in the top product ($x_{D,nc4}$). The first value of heavy component ($x_{D,nc4} = 2\%$) is defined from the setpoint for Model Predictive Control (Septic), whereas the second value ($x_{D,nc4} = 4\%$) is the specification of stream, set by the customer. The results from optimization of operation point 1 at full rate is presented in table 4.4. The values of J function were calculated with equation 3.7. These are also presented graphically in figure 4.17. The optimum operation was found to be when $x_{B,ic4} = 1\%$. That is J function reduction by the magnitude of 327.0 (3.59%) from operation on setpoint and 149.3 (1.64%) from operation at specifications.

Table 4.4: Calculation of J function in Butane Splitter with feed rate $6.5732E+04$ kg/h.

	$x_{B,ic4}$ [%]	B [kg/h]	D [kg/h]	V [kg/h]	J
$x_{D,nc4} = 2\%$	0.25	4.292E4	2.281E4	2.885E5	-8.516E3
	0.5	4.304E4	2.270E4	2.638E5	-8.710E3
	0.75	4.315E4	2.258E4	2.522E5	-8.767E3
	1	4.325E4	2.248E4	2.449E5	-8.790E3
	1.25	4.337E4	2.236E4	2.397E5	-8.780E3
	1.75	4.359E4	2.214E4	2.323E5	-8.744E3
	2.25	4.382E4	2.192E4	2.271E5	-8.697E3
	3	4.416E4	2.157E4	2.210E5	-8.573E3
$x_{D,nc4} = 4\%$	0.25	4.244E4	2.329E4	2.804E5	-8.841E3
	0.5	4.256E4	2.317E4	2.558E5	-9.024E3
	0.75	4.267E4	2.306E4	2.443E5	-9.085E3
	1	4.277E4	2.296E4	2.371E5	-9.107E3
	1.25	4.290E4	2.283E4	2.319E5	-9.098E3
	1.75	4.312E4	2.261E4	2.247E5	-9.061E3
	2.25	4.336E4	2.238E4	2.194E5	-8.997E3
	3	4.370E4	2.203E4	2.134E5	-8.879E3

Figure 4.17: Cost function as a function of impurity fraction in Debutaniser at different impurity fractions in Butane Splitter, with $p' = 1.5$.

The approximations that the ratio of prices between *i*-butane and *n*-butane is 1.5 , while ratio of prices between the feed and *n*-butane is 1 were made in figure above. A change in the former to 1.3 is presented in figure 4.18. The optimum operation was found to be when $x_{B,ic4} = 1.9\%$. That is J function reduction by the magnitude of 30.9 (0.68%) from

operation on setpoint and 227.6 (5.02%) from operation at specifications.

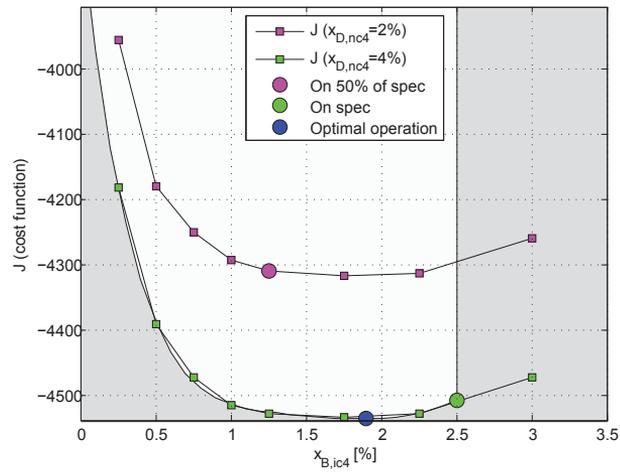


Figure 4.18: Cost function as a function of impurity fraction in Debutaniser at different impurity fractions in Butane Splitter, with $p' = 1.3$.

Chapter 5

Discussion

5.1 Comparison of the simulation programs and the plant

5.1.1 Modeling the process

Initially, in this study, modeling of the real process in Unisim was done. Some weaknesses of Unisim was found. The biggest problem was to adapt the upper parts of the columns. Coolers and condensers are different units in D-spice and the plant, this is not the case in default distillation columns in Unisim. Inserting these units and rearranging the streams resulted in misconvergence of the solvers. These units were therefore left unchanged as shown figure 3.2. This resulted in slightly different performance of pressure controllers and observed cavity in temperature controller in open loop step response during the tuning.

Another challenge in modeling part was met with reboilers. In the real plant, as well as in D-spice, heater is used separated from bottom stream, while in Unisim the bottom stream is taken out from the reboiler. One of the consequences is different location on impurity measurement in bottom stream. Which results in more buffered impurity measurement.

Regarding the plant its self, an extension of pipeline living the condenser in Propaniser should be considered. Presumed the circumstances that the dimension of the equipment in D-spice are analogous to the one in the real plant. The observation were made at full feed rate feed with 4% disturbance in major component in the feed stream, propane. The simulation is shown in figure C.2c (appendix C.1). The remarked consequence were saturation

and accordingly loss of the level controller (24_LC4036).

5.1.2 Evaluation of plant dynamics

When the dynamic model of the distillation train were created in Unisim, the dynamics in Unisim, as well as in D-spice, were to be compared with dynamics in real plant. For that reason, open loop steps in the outputs of the temperature controllers (TC) of Butane Splitter were done (Appendix A). The steps in simulation programs had the same magnitude of 1%, while in the real plant two steps were executed, with stepsize 0.5% and 0.1% at feed rate 66% and 91%, respectively. In these two responses it was expected that process gain and the delay in the reboiler should increase with reduced feed rate and consequently vapor flow in the column. This has been elaborated in section 2.3.1 with resulting equations 2.10 and 2.13, regarding the process gain and in section 2.3.2 with resulting equation 2.16, regarding the delay.

Even though the trend of increasing delay was observed to be quite close to the one expected and therefore applied in Unisim model (table 3.2), the process gain increase was observed to be rather the opposite. A possible explanation could be that steps were done with different composition in the product stream. It is also strongly suspect that simulation at 91% feed rate is done at different different pressure drop over the column. That resulted in different weir height and therefore different process gain.

5.1.3 Comparison of the dynamics

Regarding comparison of the dynamics in the real plant and the two programs, it was observed that Unisim had a more similar process gain to the real plant, than D-spice (table 3.2). As well as extrapolation and further implementation of delay in the reboiler to a real process value is much easier to achieve Unisim, rather than in D-spice.

In fact, the dynamics observed in the D-spice didn't seem to fit the real process and can therefore hardly be reliable in some of the simulations (appendix A). Presumptive explanation to that could be the fact that D-spice is operated with different tray holdup than Unisim and the plant. The correlation between vapor flow in the column and the holdup (2.13) in terms of process gain was observed exclusively in Debutaniser. Whereas in Unisim the trend was observed in the whole distillation. The data is presented in table 4.2 and 4.3, respectively.

Further recommendation would be to implement holdup variation in the models of Depropaniser and Butane Splitter as well as delay in the reboiler. The latter was found to be almost completely absent in all of three columns. Implementation of both of these recommendations would result in more accurate simulations.

Regarding the stationary effect caused by temperature differences between two adjacent trays (equation 2.10), this was found to be quite similar for both of the simulation programs with respect to Depropaniser and Debutaniser. This was not the case for Butane Splitter. Considerable temperature difference in top and bottom stage of the column, despite equivalent operation with respect to feed rate, feed composition and product composition, was observed (figure 3.5). This could be caused by thermodynamical tables in D-Spice, with reference composition diverging from existing composition.

5.2 Justification of unstable behavior

It is demonstrated, that the right tuning and profitable operation of the process will not result in oscillatory behavior of the control structure that is applied in the process (appendix C- D). This is also applied to the temperature controller. However, it is comprehensible, that operation far from original design can result in different control behavior. A retuning of some of the controllers at regular intervals could therefore be recommended.

The reason for initial instability observed in the real plant could be explained by the change in the temperature profile in the column, resulting in higher process gain. This may occur at low feed rate, when decision of which of the product streams should be held on specification which should be overpurified, is necessary to take. As it has been shown, choosing to hold bottom composition on the specifications, will in fact result in oscillatory behavior (appendix E). Supervisory layer, as MPC, may also exacerbate the control. In such cases the best solution is to retune the primary control layer or to choose different operation. This is shown in appendix F and D, respectively.

Gain scheduling is not required in this process. However, if gain scheduling, by some occurrence is contrary to expectation preferred. A good suggestion is to implement a temperature measurement in a temperature sensor near temperature controller, like for instance 24.TT4135, and this way identify the slope in temperature profile. Supervisory layer can also be supplemented with different gain regions. However, this is not essential, since MPC software (Septic) has a feedback loop for gain correction.

At least, from the temperature profile in Butane Splitter it is observed that TC location is somewhat not optimum, concerning the slope of temperature profile (figure 3.5). When that is stated, it also important to mention that in both simulation programs it is observed that oscillations smooth down in the former columns before entering Butane Splitter. A right PI tuning, done by SIMC tuning rules, will consequently not result in bigger oscillation as long as operation is kept on profitable operation.

5.3 Optimization of operation

Optimization at full rate was carried out with regard to impurity fraction of light component in the bottom product, whereas heavy component in the top product was held at two constant values. The first value is defined from the setpoint for Model Predictive Control, whereas the second value is the specification of the stream, set by the customer. As anticipated, the later is more beneficial from the economic point of view. Interpretation to that is the fact that more of the valuable product is sold this way. Further, it was assumed that most valuable product was i-butane with market price 50% higher than for n-butane. Whereas market price of n-butane was set to be the same as the feed to the column (3.4).

The result of the optimization was 1% impurity fraction of light component in the bottom product with J function reduction by 3.59% from operation on setpoint and 1.64% from operation at specifications (figure 4.17). Even though the assumption of the prices is reliable, an operation with different product prices would result in different optimum value. This has been proofed with assumed reduction of market price of i-butane to only 30% higher than for n-butane. The more equivalent price for the product resulted in higher (less profitable) cost function with smaller difference between optimal operation and operation at the specifications, with optimal operation with 1.9% impurity fraction of light component in the bottom product (figure 4.18).

The similar trend is observed with the value of the heavy component in the top product stream defined from the Septic. The recommendation is therefore an optimization unit, for example at RTO control layer. The unit should elaborate automatic optimization that consequently can supply Septic with updated setpoints, with consideration of the market prices of the products.

Operation at half rate doesn't need any type of optimization, since reflux constraint is active, and the degree of freedom is lost. Optimal operation is doubtless with distillate on specification. The profitable operation (operation point 2) is defined in such a manner.

Chapter 6

Conclusion

Comparison of the dynamics in Unisim and D-spice with the real plant revealed some weaknesses of D-spice. Even though the model in Unisim, had deficiency of the operation units with respect to convergence of the solver, the dynamic factor in the name of process gain, were found to be more appropriate in Unisim rather than D-spice. Exceptionally the dynamics in Debutaniser was found to be close to the dynamics in the plant. However, complete absent of reboiler delay was found in all of three columns.

Regarding performance elaboration of the temperature controllers in Unisim at lower feed rate, it was found that a right operation, that is also found to be the most profitable, will not result in critical unstable behavior. Holdup variation in the models of Depropaniser and Butane Splitter as well as variation in delay in all of the three reboilers was not found in D-spice. En implementation of these is strongly recommended.

Conclusion from the optimization of an impurity fraction of light component in the bottom product, resulted in somewhat lower impurity fraction of light component bottom than the specification and naturally setpoint value in Septic. In fact, J function reduction of 1.6% from specification to optimal operation was found. Consequently, a real time optimization that would consequently supply control layer below with updated setpoints, is recommended.

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Appendices

Appendix A

Comparison of the dynamics

A.1 Step in the output of TC (*24TC4113.vya*) in the real plant

Following subsection presents two open loop steps in output of the temperature controller in Butane Splitter (*24TC4113.vya*) at feed rates 66% and 91%, respectively. Step response (*24TC4113*), set point (*24TC4113.vwa*), and impurity measure in bottom stream (*24AY4139D1*, i-butane) and top stream (*24AY4170E1*) are also presented in figures A.1-A.2. Step magnitude is 0.5% and 1.0%, respectively.

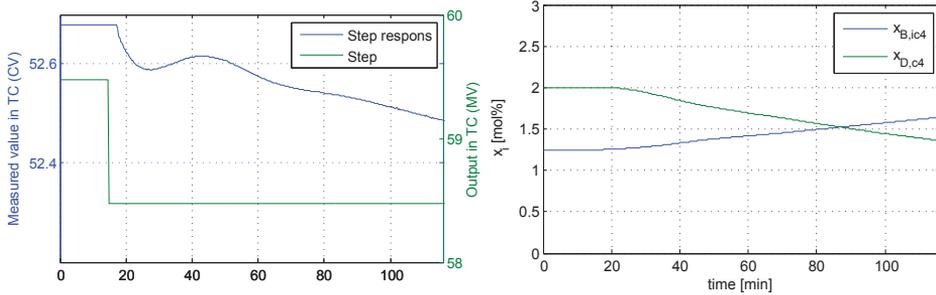


Figure A.1: Open loop step response in temperature controller at 66% feed rate with step magnitude of 0.5%. Process gain (k') and delay (Θ) are found to be 0.0267 and 2.43 min, respectively.



Figure A.2: Open loop step response in temperature controller at 91% feed rate with step magnitude of 1.0%. Process gain (k') and delay (Θ) are found to be 0.0421 and 2 min, respectively.

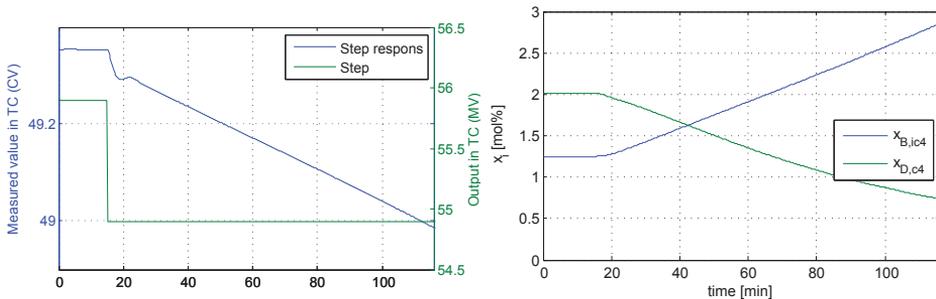
A.2 Step in the output of TC (TIC-304) in Unisim



(a) Manipulated and measured variable in the temperature controller. (b) Impurities in bottom product ($x_{B,ic4}$) and distillate ($x_{D,c4}$).

Figure A.3: Open loop step response in temperature controller at 100% feed rate with step magnitude of 1.0%. Initial process gain (k') and delay (Θ) are found to be 0.0237 and 2 min, respectively.

A.3 Step in the output of TC (24_TC4113) in D-Spice



(a) Manipulated and measured variable in the temperature controller. (b) Impurities in bottom product ($x_{B,ic4}$) and distillate ($x_{D,c4}$).

Figure A.4: Open loop step response in temperature controller at 100% feed rate with step magnitude of 1.0%. Initial process gain (k') and delay (Θ) are found to be 0.0989 and 0.17 min, respectively.

Appendix B

Tuning results for the controllers

In this section there are presented results from the tuning of the controllers with $\tau_1 \ll 4(\tau_c + \Theta)$ at full feed rate, both in Unisim (B.1) and D-spice (B.2).

Table B.1: Tuning results at full feed rate in Unisim. The delay values in brackets are the values used in transfer function block.

Column	Controller	Process		Control		
		Θ [min]	k'	τ_c [min]	K_c^*	τ_I [min]*
Depropaniser	FIC-100	0	-	-	0.0249	1
	LIC-102	0	0.5353	3	0.6227	12
	LIC-103	0	0.4257	3	0.7797	12
	TIC-104	2.00 (1.54)	0.1699	5	0.8408	28
Debutaniser	FIC-200	0	-	-	0.0310	1
	LIC-202	0.03	0.4114	3	0.8022	12.12
	LIC-203	0.03	0.2874	3	1.1483	12.12
	TIC-204	2.00 (1.36)	0.1725	5	0.8282	28
Butane splitter	FIC-300	0	-	-	0.0382	1
	LIC-302	0	0.1441	3	2.3132	12
	LIC-303	0.02	0.4074	3	0.8128	12.08
	TIC-304	2.00 (1.60)	0.0237	5	6.0277	28

Table B.2: Tuning results at full feed rate in D-spice. Parameters marked with * are used in the controllers. Controllers marked with ' are in cascade with temperature controllers.

Column	Controller	Process		Control			
		Θ [min]	k'	τ_c [min]	K_c^*	τ_I [min]	τ_I [s]*
Depropaniser	24_FC4018 (reflux)	0	-	-	0.02	0.50	30
	24_LC4036 (condenser)	0.6	0.3869	1.50	1.2308	8.40	504
	24_LC4021 (sump)	0.6	0.3978	1.50	1.1971	8.40	504
	24_LC4003' (reboiler)	0	1.1952	0.25	3.3467	1.00	60
	24_TC4008 (11-th stage)	0.17	0.7054	2.50	0.5309	10.68	641
Debutaniser	24_FC4074 (reflux)	0	-	-	0.1550	2.00	120
	24_LC4102 (condenser)	0.05	0.1062	3.00	3.087	12.00	720
	24_LIC4067 (sump)	0	0.7917	2.00	0.6316	8.00	480
	24_LC4055' (reboiler)	0	0.1835	0.50	10.899	2.00	120
	24_TIC4062 (6-th stage)	0.20	0.2474	4.00	0.9624	16.80	1008
Debutaniser	24_FC4138 (reflux)	0	-	-	0.3263	0.5	30
	24_FIC4129' (reboiler)	0	-	-	0.9947	0.5	30
	24_LIC4180 (condenser)	0.20	0.0253	3.00	12.352	12.80	768
	24_LC4132 (sump)	0.33	0.0527	2.00	8.1439	9.32	559
	24_LC4125 (reboiler)	0.03	0.2640	0.50	7.147	2.12	127
	24_TC4113 (7-th stage)	0.17	0.0989	4.00	2.4248	16.68	1001

Appendix C

Simulation at full rate

C.1 Depropaniser

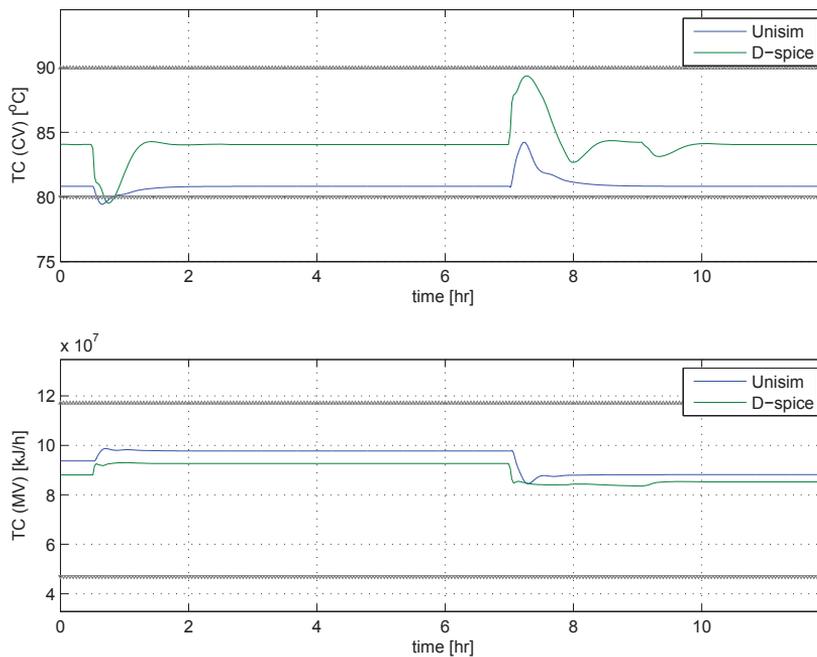


Figure C.1: Behavior of manipulated and controlled variables for temperature controller at full rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

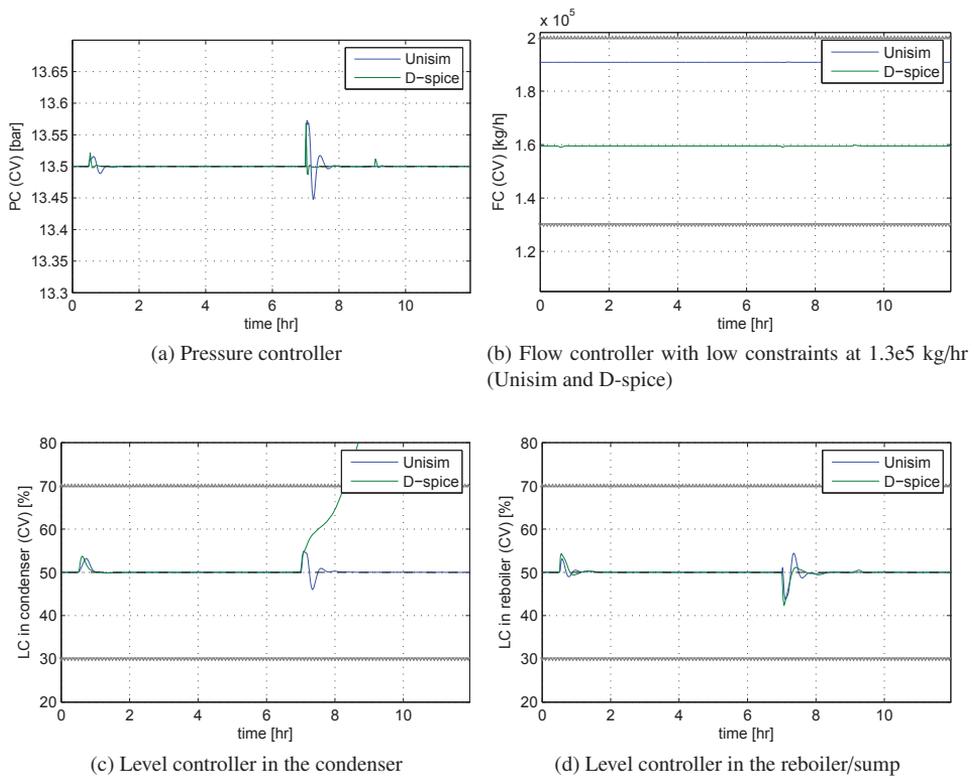


Figure C.2: Behavior of controlled variables in the controllers at full rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

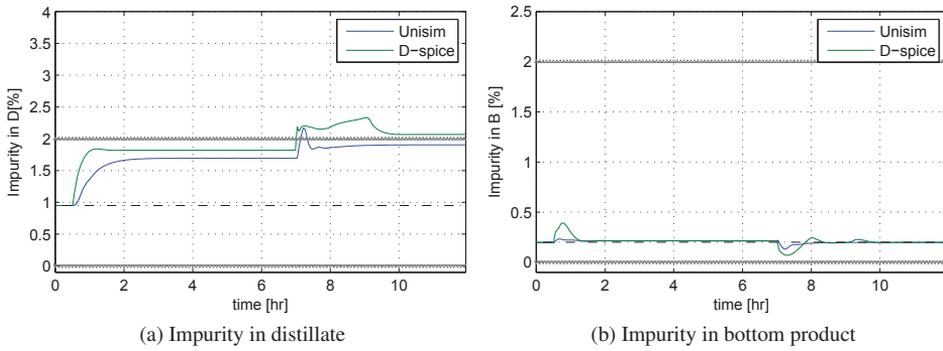


Figure C.3: Impurities in distillate and bottom product at full rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

C.2 Debutaniser

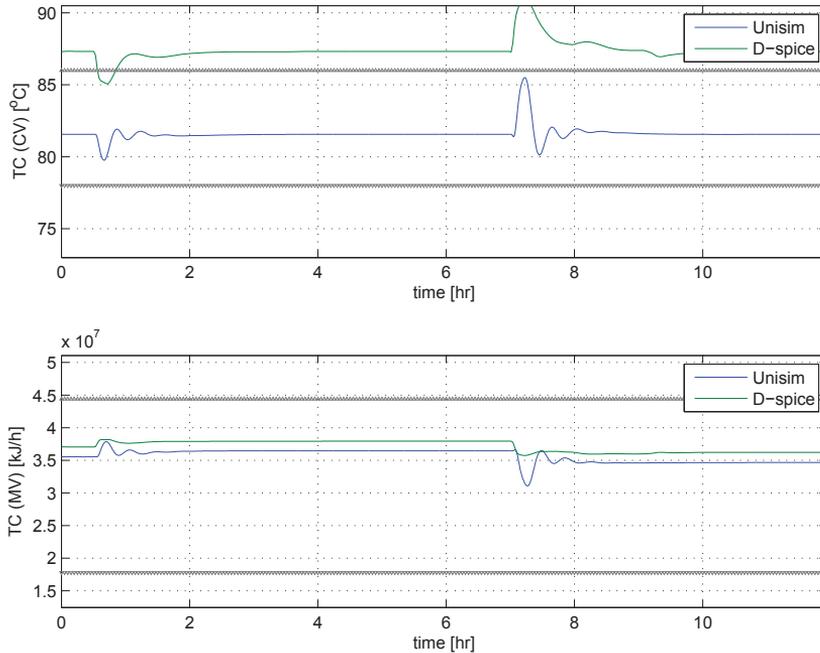


Figure C.4: Behavior of manipulated and controlled variables for temperature controller at full rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

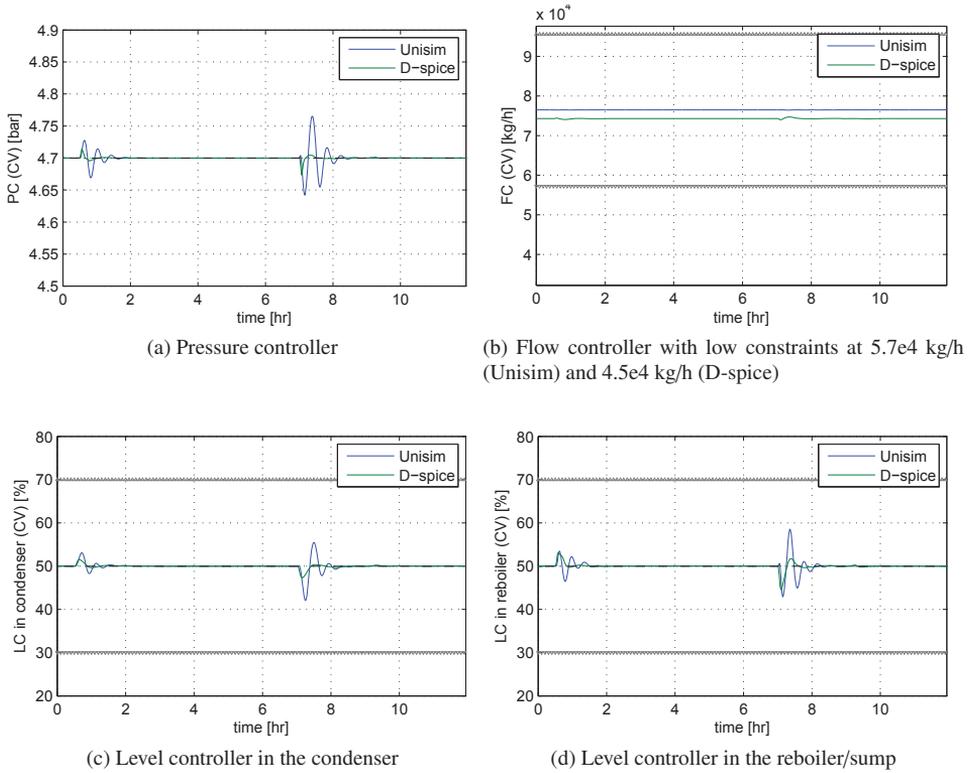


Figure C.5: Behavior of controlled variables in the controllers at full rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

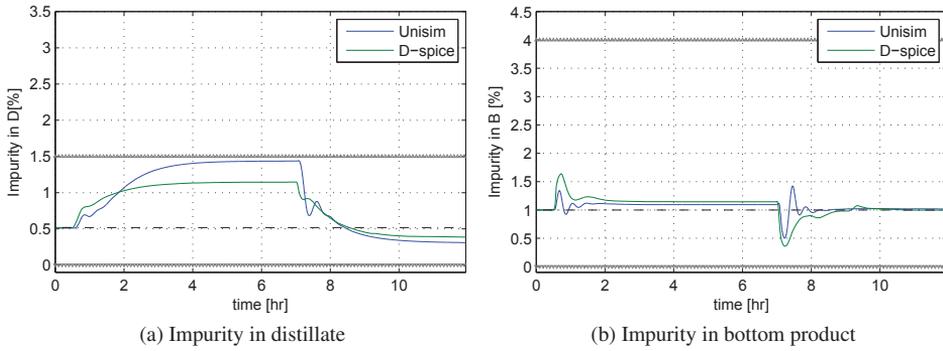


Figure C.6: Impurities in distillate and bottom product at full rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

C.3 Butane splitter

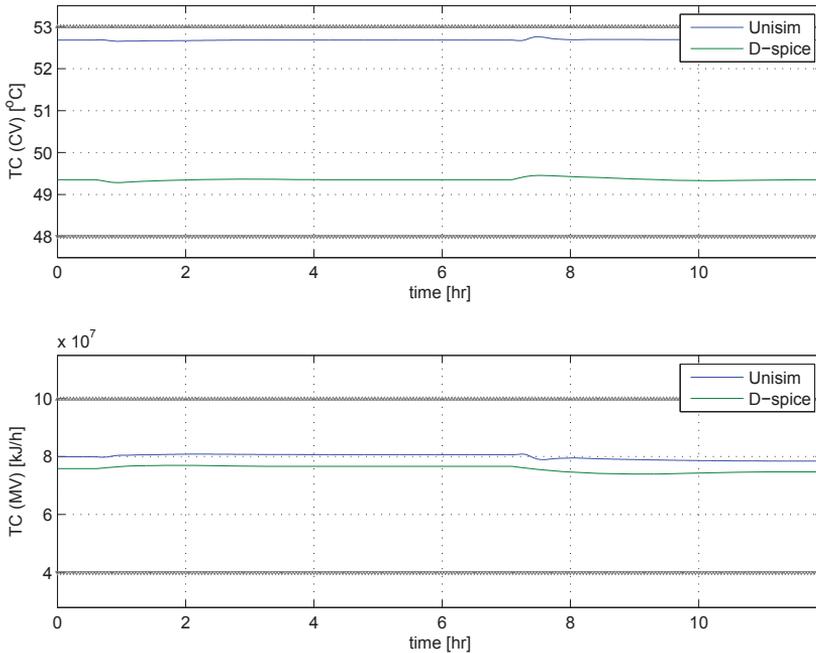


Figure C.7: Behavior of manipulated and controlled variables for temperature controller at full rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

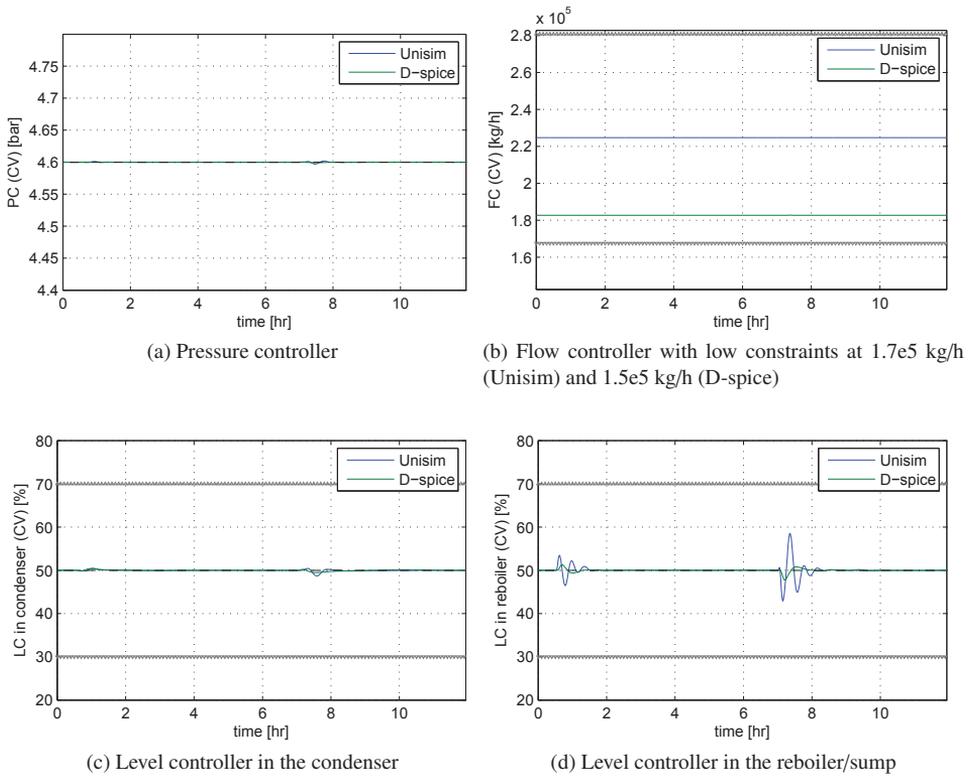


Figure C.8: Behavior of controlled variables in the controllers at full rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

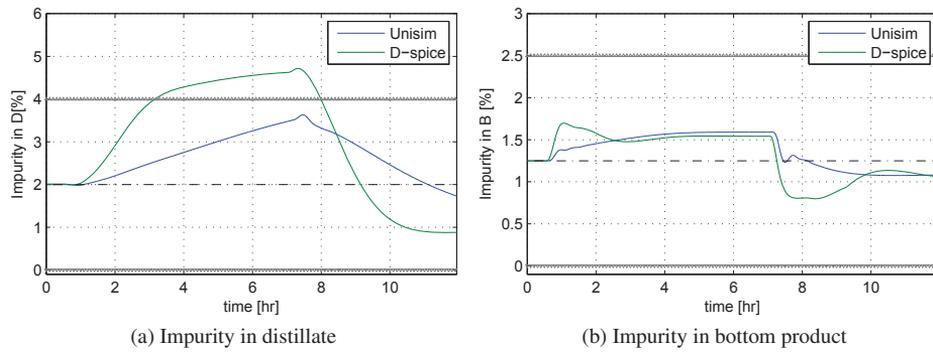


Figure C.9: Impurities in distillate and bottom product at full rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

Appendix D

Simulation at half rate, profitable operation

D.1 Depropaniser

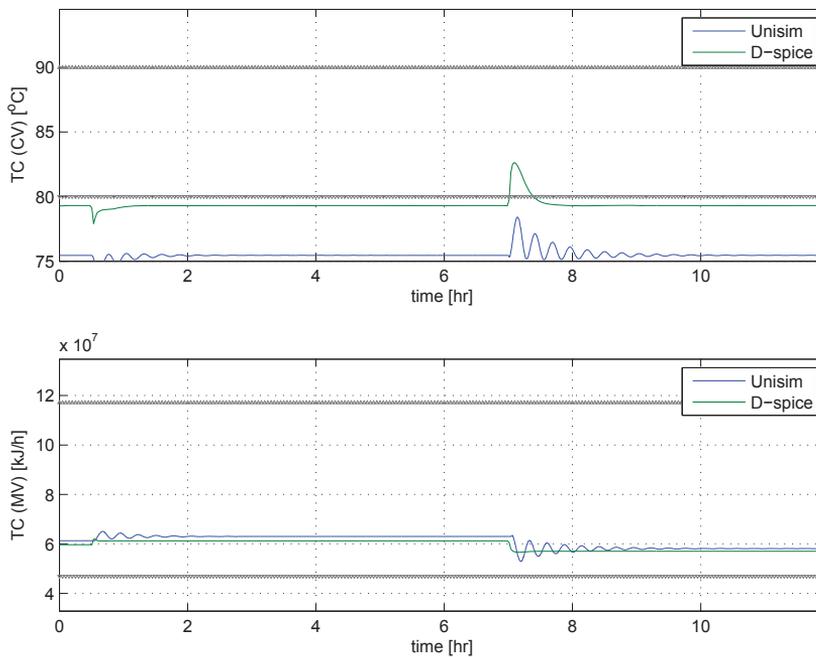


Figure D.1: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

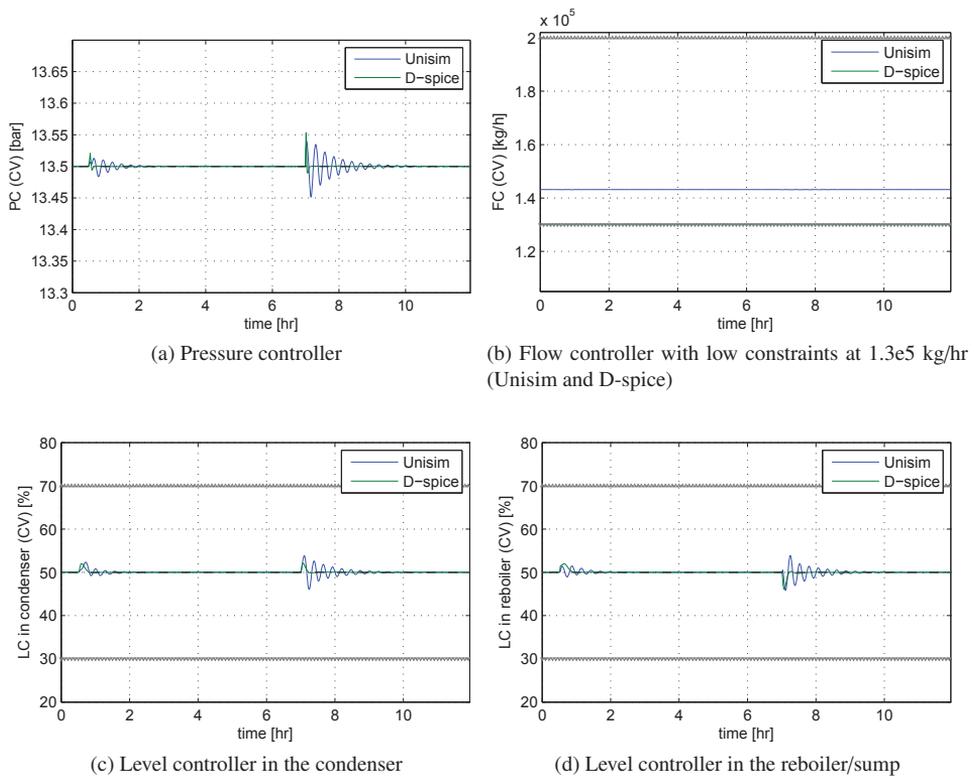


Figure D.2: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

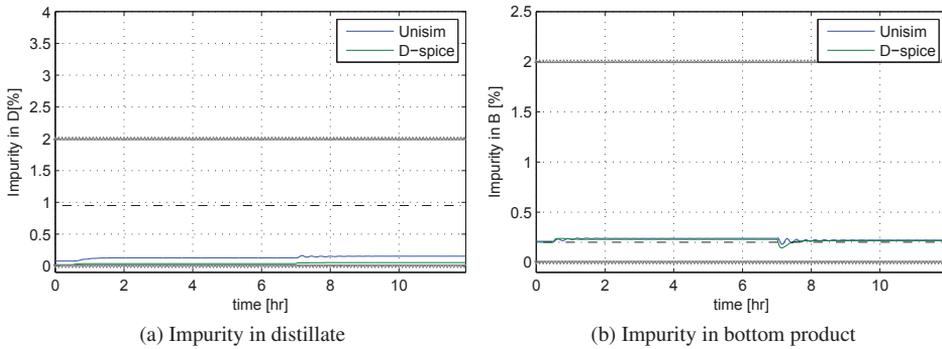


Figure D.3: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

D.2 Debutaniser

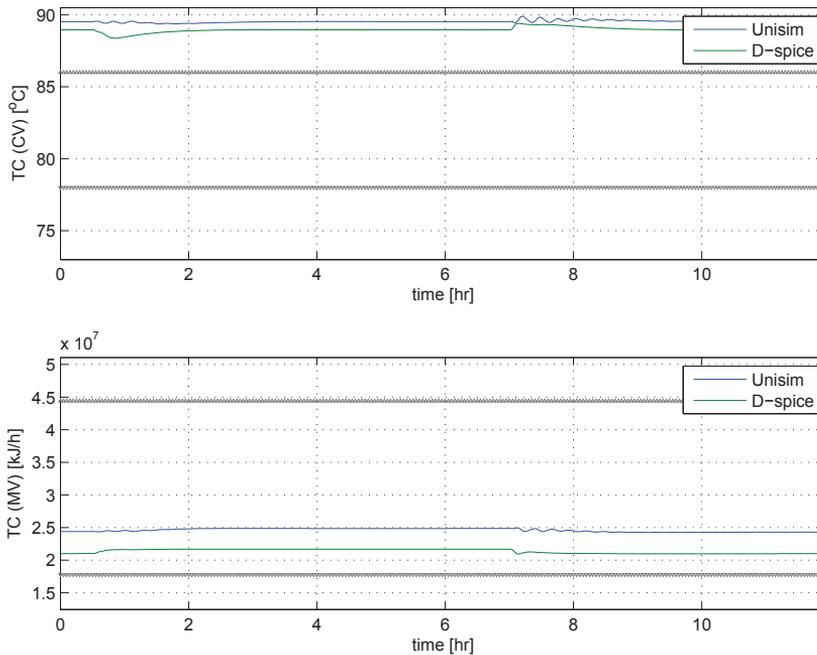


Figure D.4: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

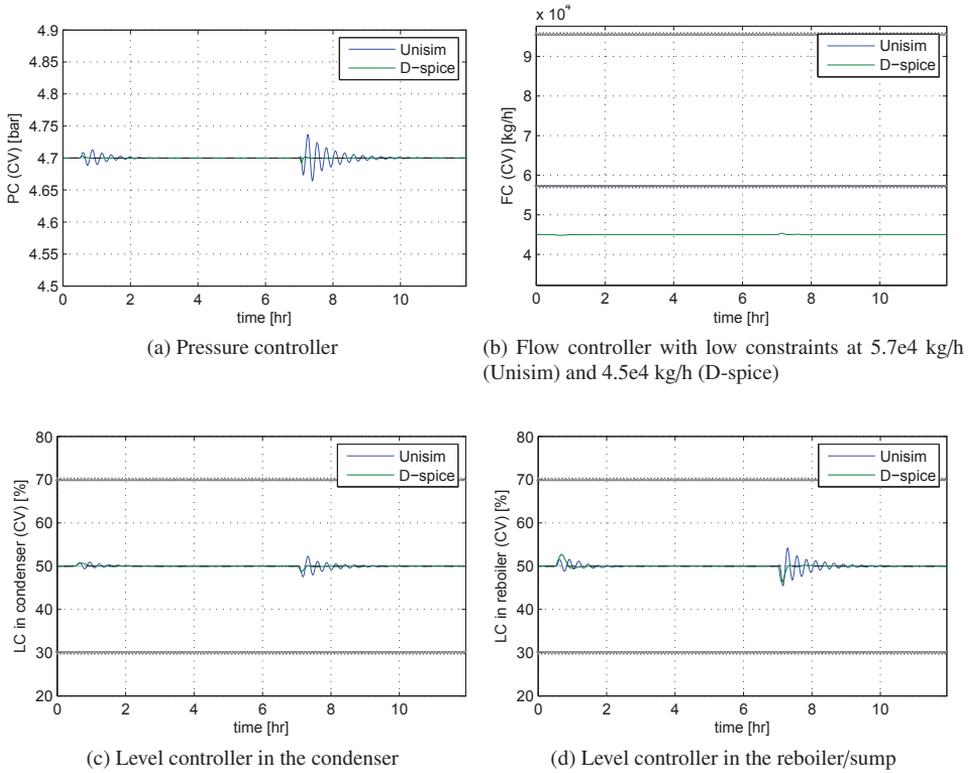


Figure D.5: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

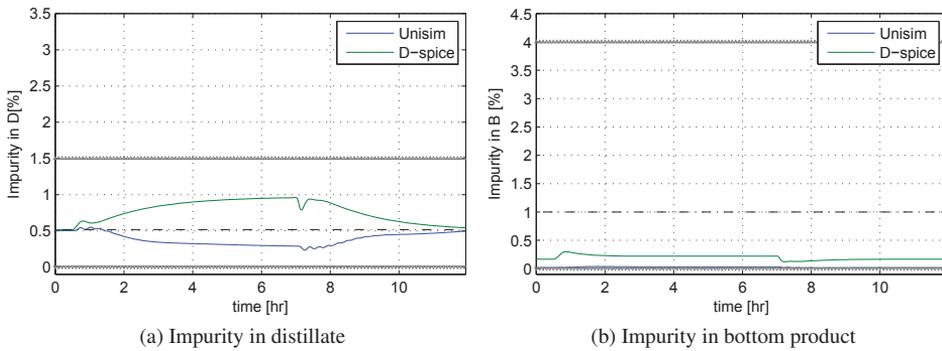


Figure D.6: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

D.3 Butane splitter

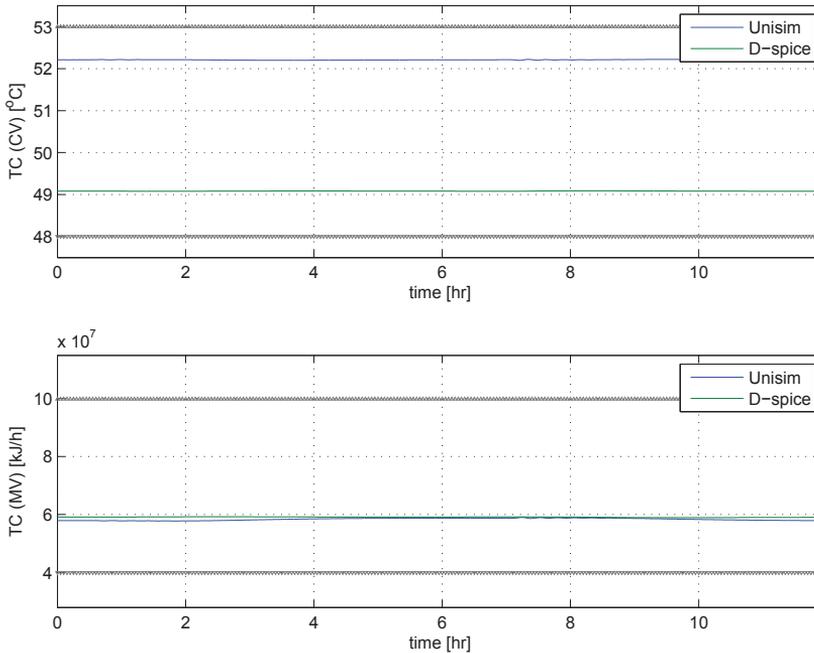


Figure D.7: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

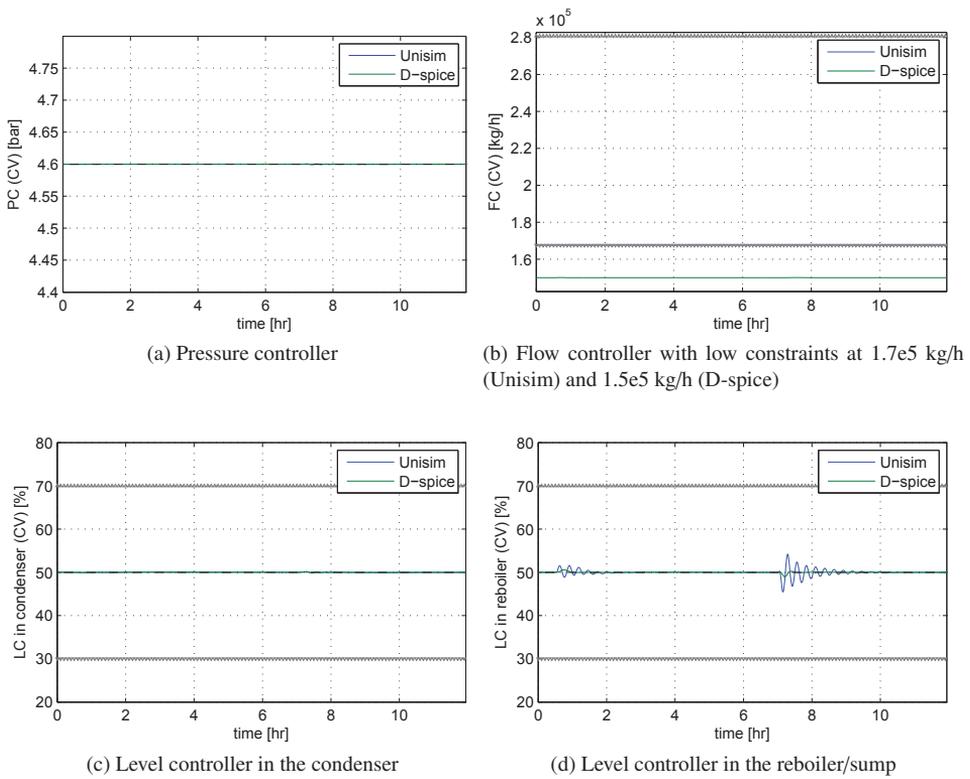


Figure D.8: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

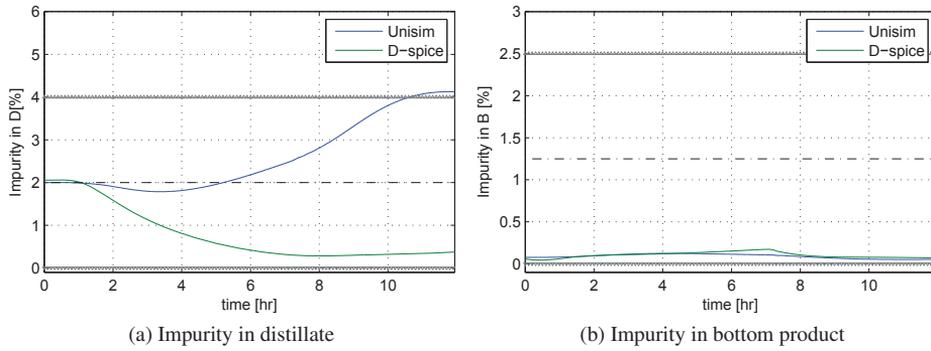


Figure D.9: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

Appendix E

Simulation at half rate, nonprofitable operation

E.1 Depropaniser

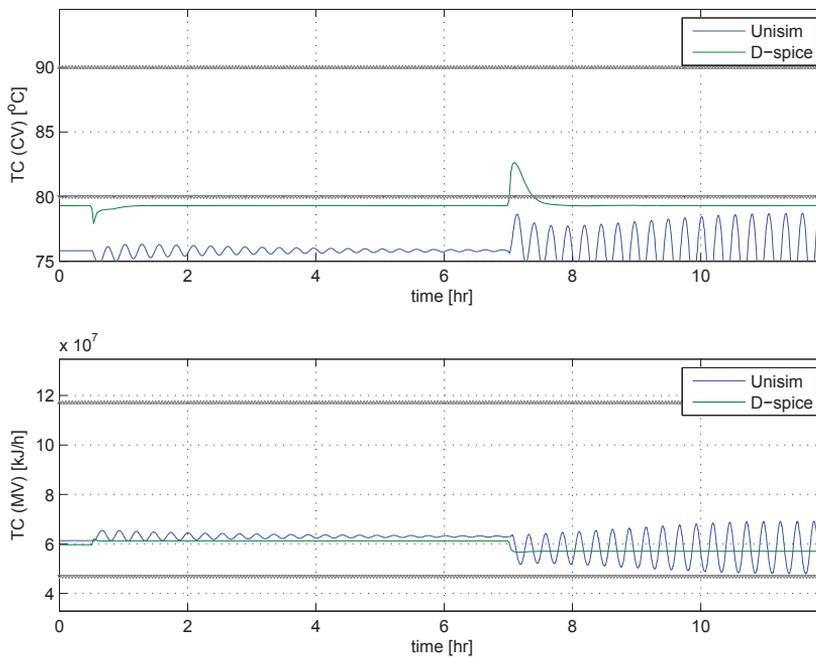


Figure E.1: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

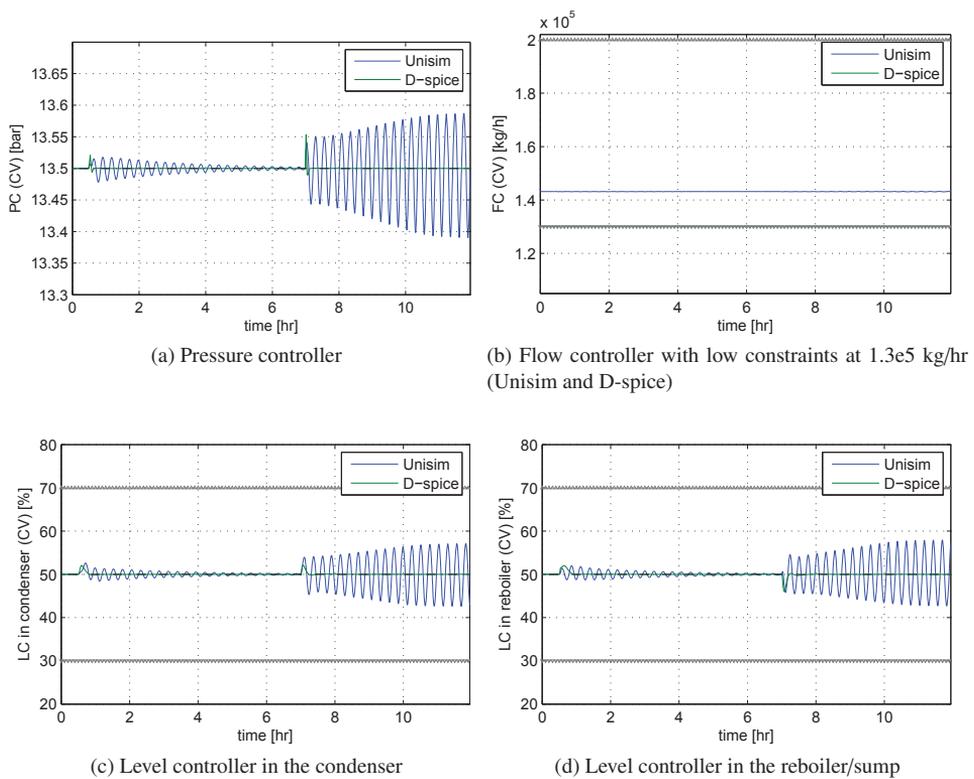


Figure E.2: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

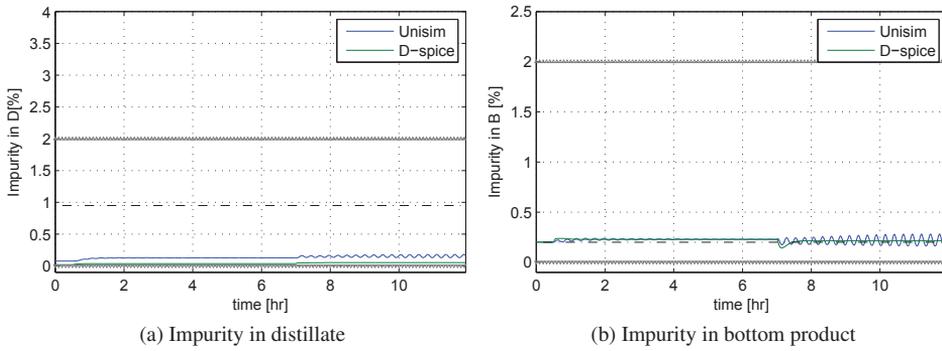


Figure E.3: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

E.2 Debutaniser

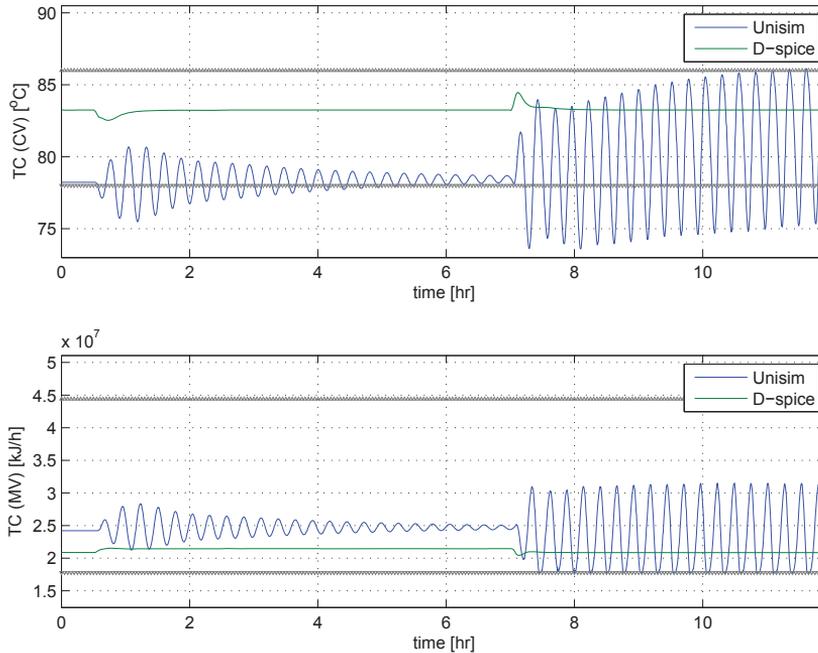


Figure E.4: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

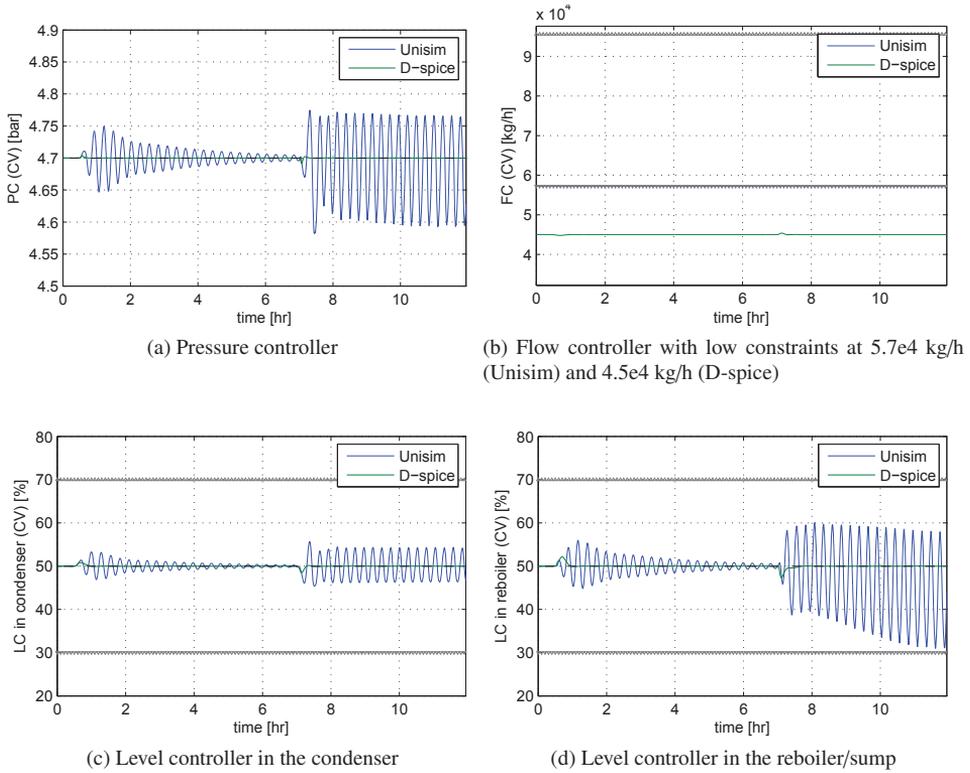


Figure E.5: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

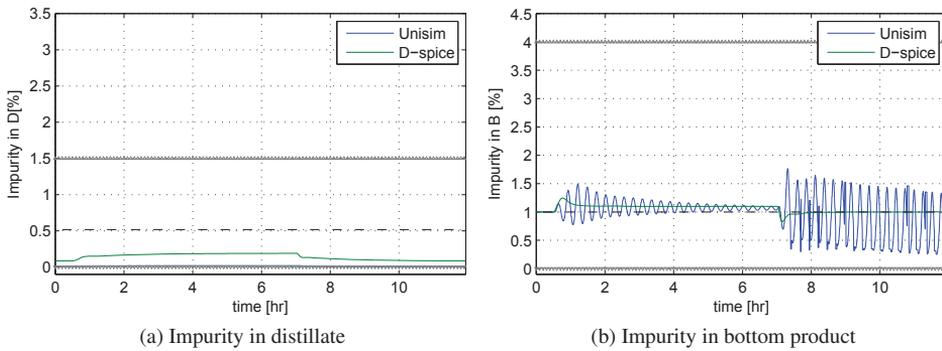


Figure E.6: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

E.3 Butane splitter

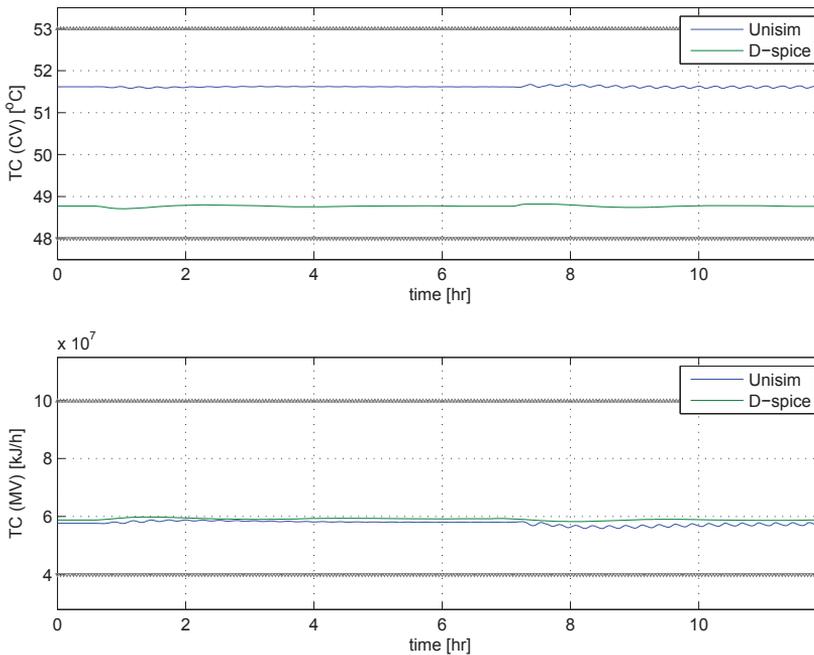


Figure E.7: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

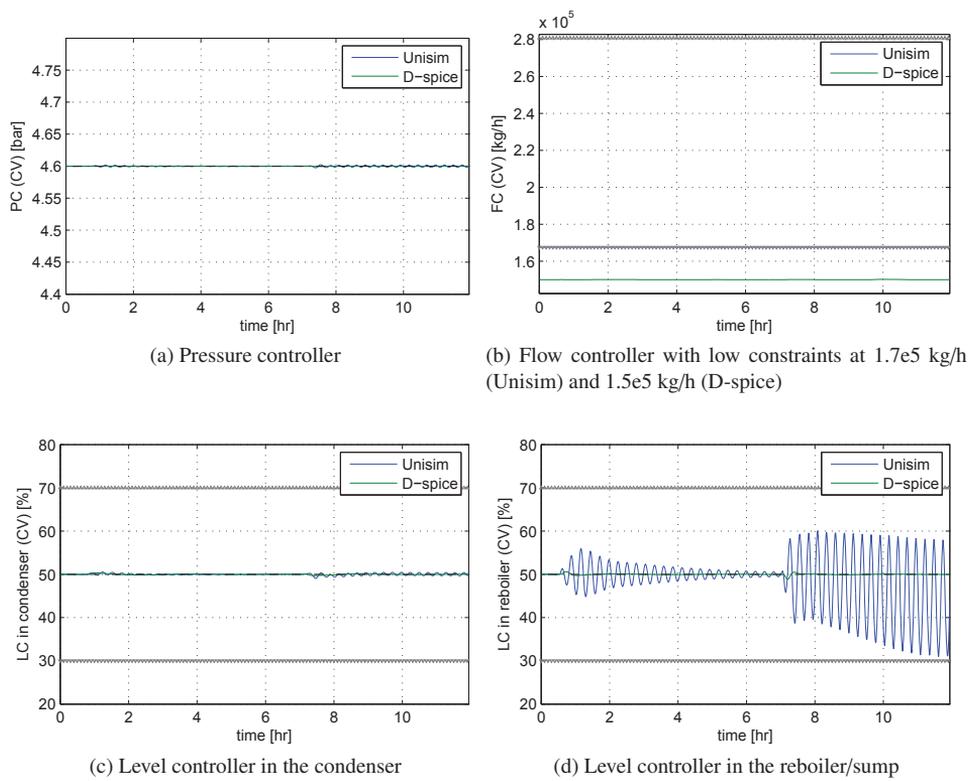


Figure E.8: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

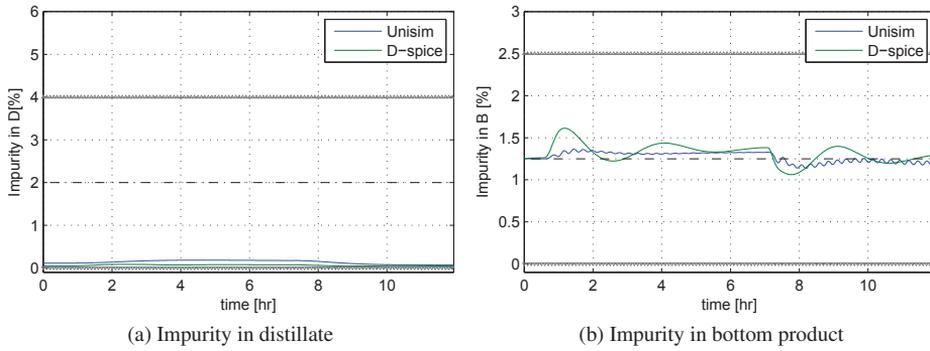


Figure E.9: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

Appendix F

Simulation at half rate, nonprofitable operation, retuned

Following simulation results are obtained with TC retuned at current operation point. All of the other controllers have PI controller parameters sustained from operation point 1.

F.1 Depropaniser

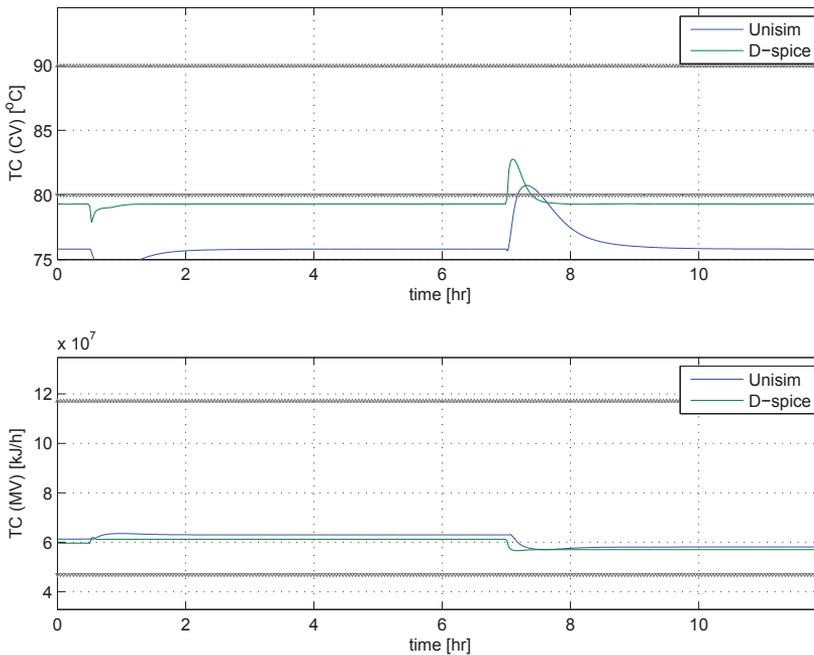


Figure F.1: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

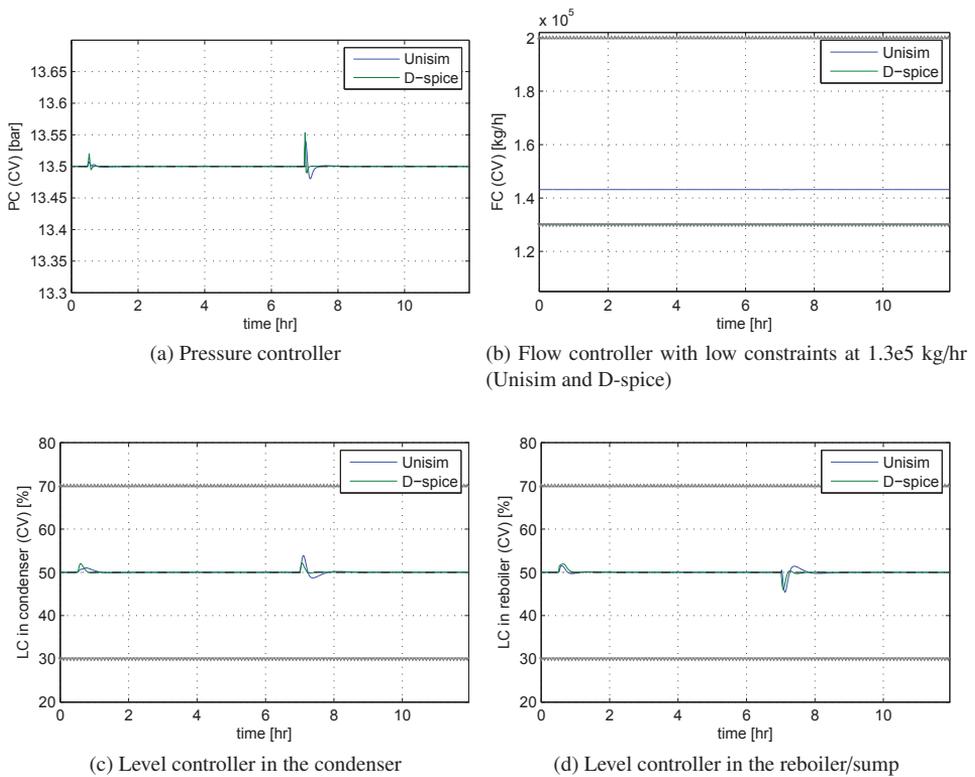


Figure F.2: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

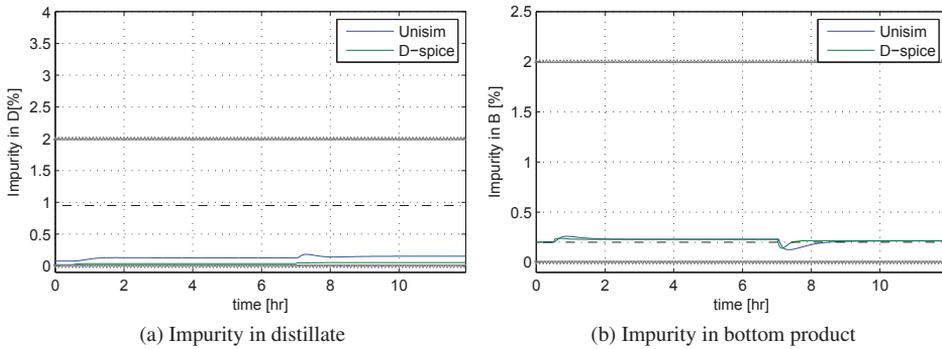


Figure F.3: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

F.2 Debutaniser

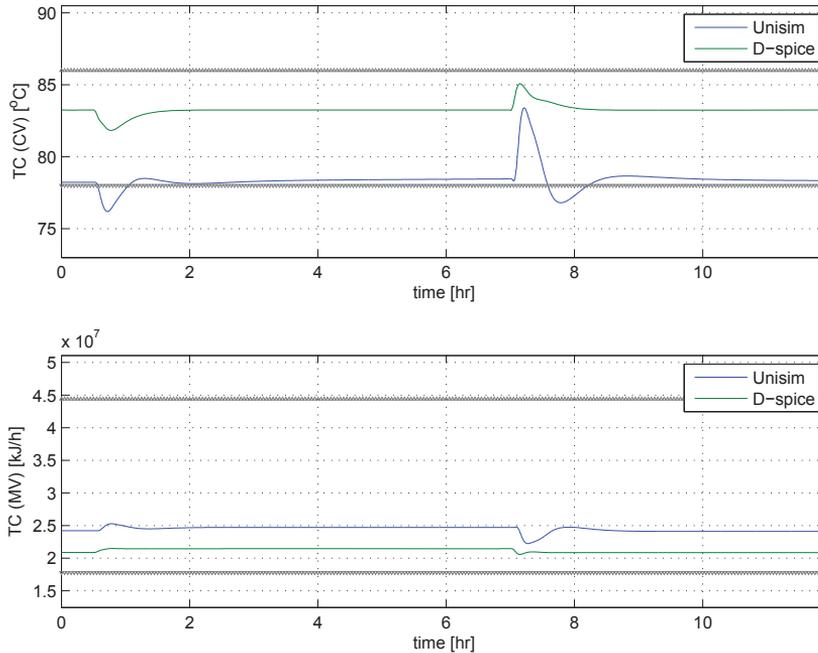


Figure F.4: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

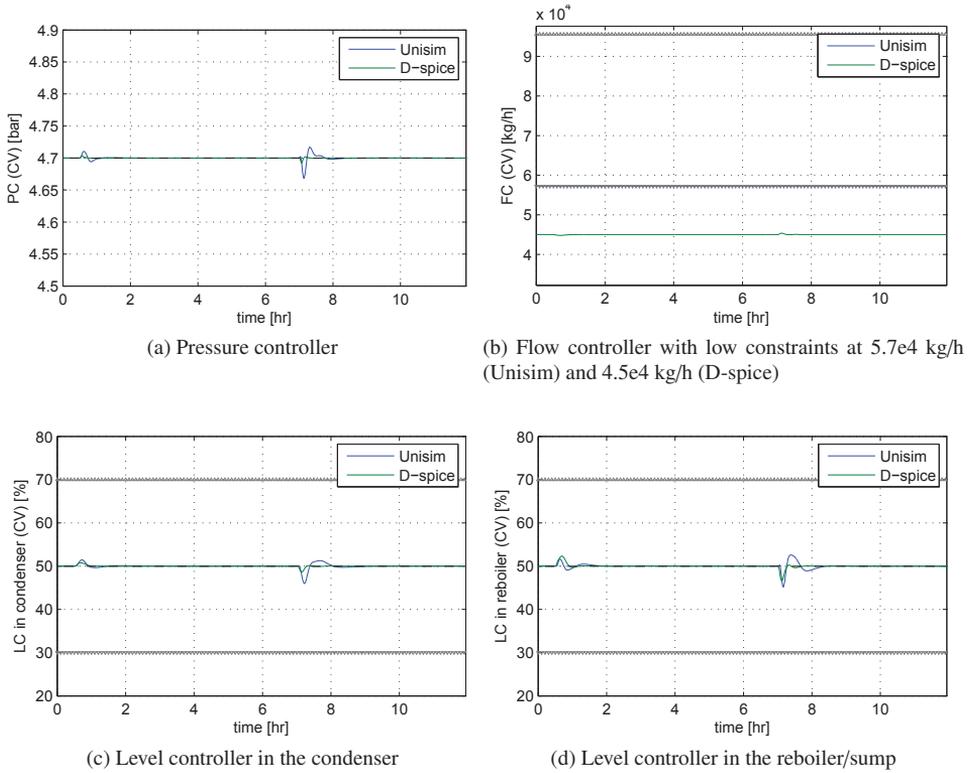


Figure F.5: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

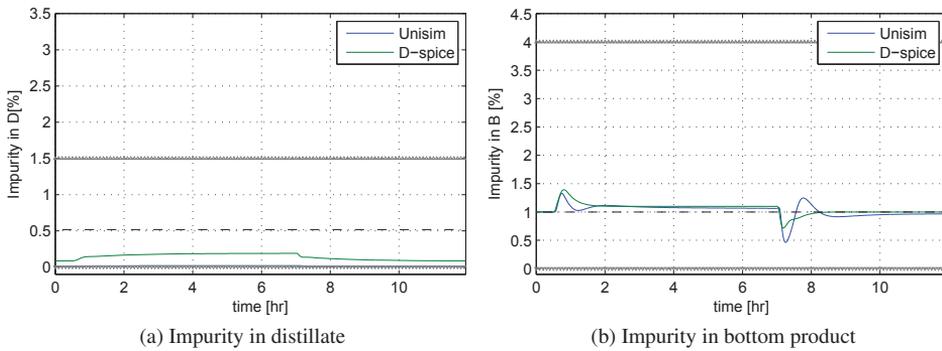


Figure F.6: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

F.3 Butane splitter

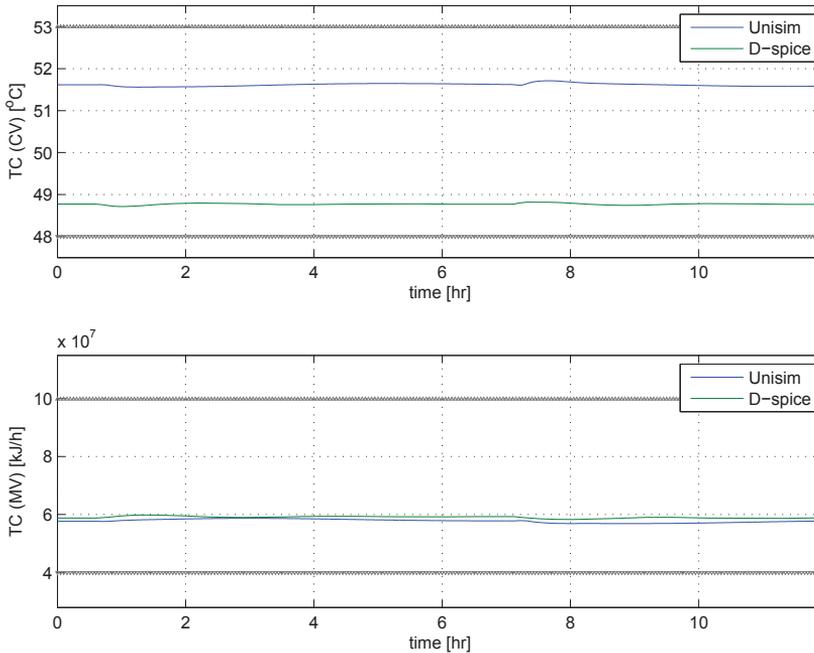


Figure F.7: Behavior of manipulated and controlled variables for temperature controller at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

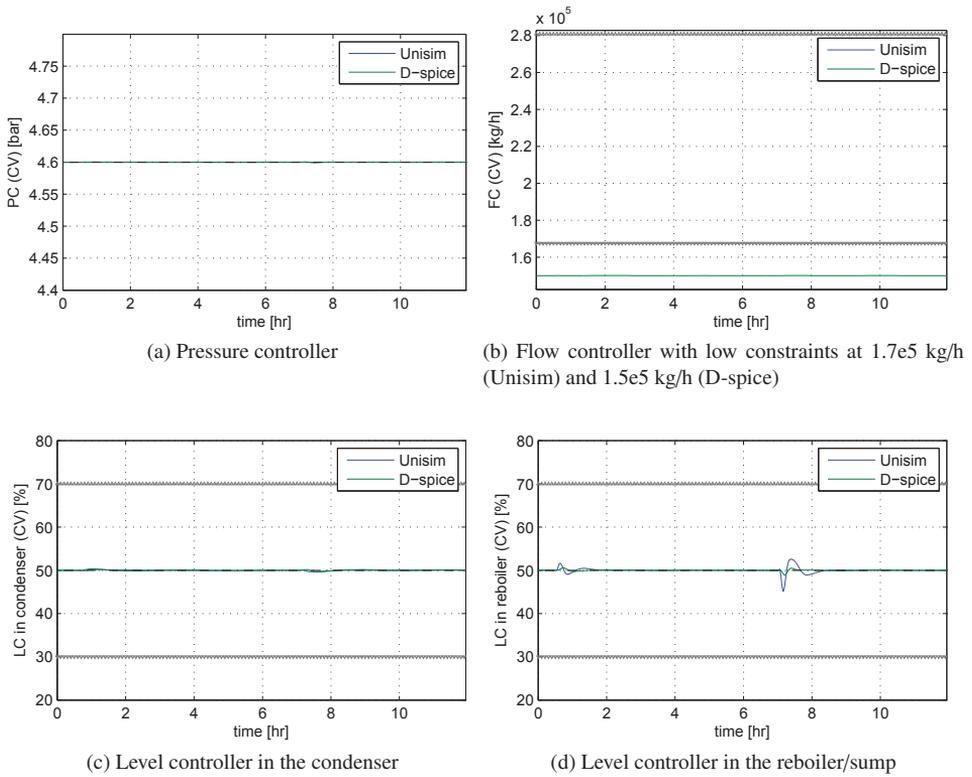


Figure F.8: Behavior of controlled variables in the controllers at half rate with disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

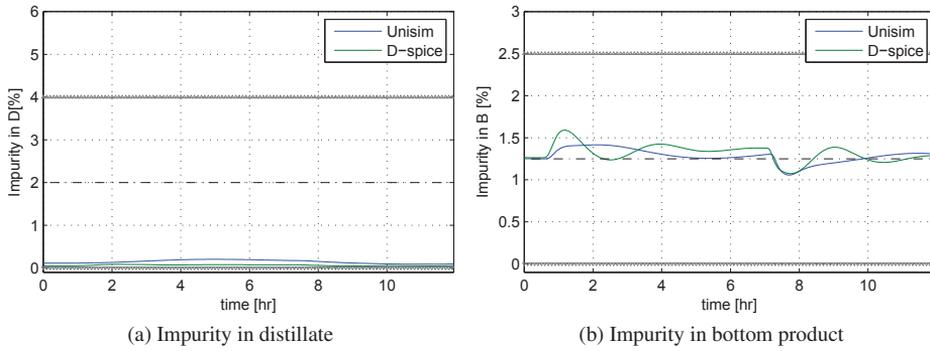


Figure F.9: Impurities in distillate and bottom product at half rate as a result of disturbance in feed rate ($dF = 10\%$) after 0.5 hour and feed composition ($dzF_{Propane} = 4\%$) after 7 hours.

Appendix G

Matlab code

In following section, some of the Matlab files are presented.

G.1 Superior Matlab code

Together with *importfile.m* (G.2) and *importfile_unisim.m*(G.3) the following Matlab code was used to illustrate the performance of the controllers in the process. First of all, simulation programs were operated for 12 hours, then the data was imported and processed by the specified scripts. Finally data was plot and saved.

```
%-----%
%----- The file is used to define constraints , -----%
%----- import data with "importfile.m" (from D-spice) and -----%
%----- "importfile_unisim.m" (from Unisim) -----%
%----- and plot the simulation data -----%
%-----%

clc
clf
clear all;
close all;

%Import '.csv' files from Unisim and '.txt' from D-Spice:

%Operation point 1
data_uni=importfile_unisim('Data_Unisim_fullrate.csv');
```

```

data= importfile('Data_D-Spice_fullrate.txt');

%Operation point 2
%data_uni=importfile_unisim('Data_Unisim_halftrate_prof.csv');
%data= importfile('Data_D-Spice_halftrate_prof.txt');

%Operation point 3
%data_uni=importfile_unisim('Data_Unisim_halftrate_nonprof.csv');
%data= importfile('Data_D-Spice_halftrate_nonprof.txt');

%Operation point 3, retuned
%data_uni=importfile_unisim('Data_Unisim_halftrate_nonprof_retuned.csv');
%data= importfile('Data_D-Spice_halftrate_nonprof_retuned.txt');

% Define time from D-spice
D_time_min=data(:,1)/60;
D_time_hr=data(:,1)/60/60;

%%
%Define limits

%TC
TC_CV=[80 90;
       78 86;
       48 53]; %from Unisim
TC_MV=[4.6865e7 1.1716e8;
       1.7763E+07 4.4407E+07;
       3.9933E+07 9.9834E+07]; %Self defined

%Product streams
Comp_limit_D=[0 2;
              0 1.5;
              0 4];
Comp_set_D=[0.95; 0.518; 2];
Comp_limit_B=[0 2;
              0 4;
              0 2.5];
Comp_set_B=[0.2; 1; 1.25];

%PC
PC1_set= [13.5; 4.7; 4.6];

%FC
FC_limit= 10^5*[1.3 2.0; %min--> Septic ~ = Unisim
               0.572 0.956; %min--> Septic (4.5e4) < Unisim(5.72e4)
               1.675 2.808]; %min--> Septic (1.5e5) < Unisim(1.675e5)

%LC
LC_limit=[30 70;
          30 70;
          30 70];
LC_set=[50; 50; 50];

```

```
%First and last time measure
t=[time_hr(1) time_hr(end)];
t1=t(1):0.05:t(2); %used to draw constraints for TC
t12=t(1):0.1:t(2); %used to draw constraints for all of the other controllers

%%
%Generate the plots
Plotter

%Save the plots
Saver
```

G.2 Function that imports data from D-spice

```
function [data]= importfile(fileToRead1)
%IMPORTFILE(FILETOREAD1)
% Imports data from the specified file
% FILETOREAD1: file to read

DELIMITER = '\t';
HEADERLINES = 35;

% Import the file
newData1 = importdata(fileToRead1, DELIMITER, HEADERLINES);

% Create new variables in the base workspace from those fields.
data=newData1.data;
end
```

G.3 Function that imports data from Unisim

```

function [data_uni] = importfile_unisim (fileToRead1)
d = csvread (fileToRead1,11,0);
last= length(d);

%Time
time = csvread (fileToRead1,11,0, [11,0,last,0]);

%Depropaniser
data_uni.FIC_100 = csvread (fileToRead1,11,1, [11,1,last,2]);
data_uni.LIC_102 = csvread (fileToRead1,11,3, [11,3,last,4]);
data_uni.LIC_103 = csvread (fileToRead1,11,5, [11,5,last,6]);
data_uni.PIC_101 = csvread (fileToRead1,11,7, [11,7,last,9]);
data_uni.TIC_104 = csvread (fileToRead1,11,10, [11,10,last,12]);
Comp1 = csvread (fileToRead1,11,13, [11,13,last,14]);

%Debutaniser
data_uni.FIC_200 = csvread (fileToRead1,11,15, [11,15,last,16]);
data_uni.LIC_202 = csvread (fileToRead1,11,17, [11,17,last,18]);
data_uni.LIC_203 = csvread (fileToRead1,11,22, [11,22,last,23]);
data_uni.PIC_201 = csvread (fileToRead1,11,19, [11,19,last,21]);
data_uni.TIC_204 = csvread (fileToRead1,11,24, [11,24,last,26]);
Comp2 = csvread (fileToRead1,11,27, [11,27,last,28]);

%Butane splitter
data_uni.FIC_300 = csvread (fileToRead1,11,29, [11,29,last,30]);
data_uni.LIC_302 = csvread (fileToRead1,11,31, [11,31,last,32]);
data_uni.LIC_303 = csvread (fileToRead1,11,36, [11,36,last,37]);
data_uni.PIC_301 = csvread (fileToRead1,11,33, [11,33,last,35]);
data_uni.TIC_304 = csvread (fileToRead1,11,38, [11,38,last,40]);
Comp3 = csvread (fileToRead1,11,41, [11,41,last,42]);

%Sorting the data
data_uni.time_s=time(:,1);
data_uni.time_min=time/60;
data_uni.time_hr=time/60/60;

data_uni.Comp1_D=Comp1(:,1)*100; %converting to per cent
data_uni.Comp1_B=Comp1(:,2)*100; %converting to per cent
data_uni.Comp2_D=Comp2(:,1)*100; %converting to per cent
data_uni.Comp2_B=Comp2(:,2)*100; %converting to per cent
data_uni.Comp3_D=Comp3(:,1)*100; %converting to per cent
data_uni.Comp3_B=Comp3(:,2)*100; %converting to per cent

vars = fieldnames(data_uni);
for i = 1:length(vars)
    assignin('base', vars{i}, data_uni.(vars{i}));
end

```