# Modelling and Optimization of a Two-Stage Compressor Train

Adriaen Verheyleweghen, (verheyle@stud.ntnu.no)

Supervisors: Sigurd Skogestad & Johannes Jäschke

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# Abstract

A model for a two-stage refrigeration cycle was implemented in MATLAB. Dynamic simulations were done to verify the model. The model was optimized at steady state to minimize the energy consumption and the nominal operating point was found. It was found that the model had no unconstrained degrees of freedom left. An alternative case were it was attempted to maximize the heat transfer, was also studied.

# Contents

List of Figures

List of Tables

# List of Symbols

Symbol	Explanation		
$\gamma_{avg}$	Adiabatic ratios. Average ratio between specific heats, [-] Corresponding variable in script: POL		
$\delta_i$	Coefficients for calculating HFL as a function of temperature.		
$\zeta_i$	Coefficients for calculating HFG as a function of temperature.		
$\eta$	Polytropic efficiency of compressor, [-]		
$\lambda_i$	Coefficients for calculating $\nu$ as a function of temperature.		
ν	Liquid specific volume, $[m^3/kg]$		
$\phi_i$	Coefficients for calculating z as a function of temperature		
А	Constant in the Antoine equation		
В	Constant in the Antoine equation		
С	Constant in the Antoine equation		
$\mathbf{C}_i$	Constants for calculating CP as a function of temperature		
$C_{ii}$	Constants for compressor curves		
CP	Heat capacity, [J/kg K]		
CV	Valve constant, $[kg/s\sqrt{bar}]$		
$\mathbf{e}_i$	Constants for compressor curves		
FCP	Product of flow rate and heat capacity of external cooling stream, $[\mathrm{W}/\mathrm{K}]$		
FG	Mass flow of vapour stream, [kg/s]		
FGCD	Discharge flow rate of vapour out of the compressor, [kg/s]		
FGCS	Suction flow rate of vapour in to the compressor, [kg/s]		
FGV	Volumetric flow rate of vapour into compressor, $[m^3/s]$ (Corresponding variable in script: FGS)		
$\mathrm{FL}$	Mass flow of liquid stream , $[kg/s]$		
g	Gravitational constant, $[m/s^2]$		
h	Compressor head, [m] (Corresponding variable in script: HH)		
hs	Scaled compressor head, [m] (Corresponding variable in script: HS)		
Н	Enthalpy in the tank, [J]		
HFL	Specific enthalpy of the liquid stream, [J/kg]		
HFG	Specific enthalpy of the vapour stream, [J/kg]		
k	Polytropic constant, [-] (Corresponding variable in script: G)		
$M_{\rm w}$	Molecular weight, [kg/mol]		
Ν	Fractional compressor speed based on normal operation, [-]		
р	Constant in compressor curve. Value depends on compressor.		
Р	Pressure in tank, [bar]		

PS	Suction pressure, [bar]
q	Constant used in compressor curve. Value depends on compressor.
Q	Heat transferred in evaporator or condenser, [W]
R	Universal gas constant, [J/K mol]
Т	Temperature in tank, [°C]
TD	Discharge temperature from compressor, [°C]
TPI	Inlet temperature of process stream to evaporator or condenser, [°C]
ТРО	Outlet temperature of process stream from evaporator or condenser, $[^\circ \mathrm{C}]$
TS	Interstage mixing temperature / suction temperature into the compressor, $[^\circ\mathrm{C}]$
UA	Product of heat transfer coefficient and heat transfer area for a heat exchanger, $\left[\mathrm{W}/\mathrm{K}\right]$
V	Volume of the tank $[m^3]$
VG	Specific volume of vapour refrigerant, $[m^3/kg]$
W	Mass accumulated in tank, [kg]
WL	Liquid inventory in tank, [kg]
WLV	Volumetric liquid inventory in tank, [m <sup>3</sup> ]
WV	Vapour inventory in tank, [kg]
XV	Fractional valve opening of valve, also used to refer to the valve itself, [-]
Z	Compressability factor, [-]

# List of Abbreviations

## Abbreviation Explanation

CV	Controlled variable
DAE	Differential algebraic equation
DOF	Degrees of freedom
HP	High pressure
IP	Intermediate pressure
LP	Low pressure
MV	Manipulated variable
SS	Steady-state
TPM	Throughput manipulator

## 1 Introduction

This report is the final product of a project on 'Modelling and Optimization of a Two-Stage Compressor Train'. The projected was conducted by Adriaen Verheyleweghen under supervision of Johannes Jäschke and Sigurd Skogestad.

The aim of this project is to model and simulate a two-stage refrigeration cycle. The finished model is to be optimized and a control structure will be proposed to keep the plant at optimal operating conditions despite disturbances. It will be attempted to come up with a self-optimizing control structure. The model will largely be based on previous work done by Basel Asmar [4]. The model will be implemented in MATLAB.

The report is divided into three parts. The first part contains some background theory on optimizing control. The main part of the report summarizes the results from the modelling work, including the dynamic behaviour of the model, the optimal operating conditions given the defined constraints and the self-optimizing control structure. The final section contains a discussion of the results. Additional material such as MATLAB code is placed in the appendix.

### 1.1 Process description

The process flow diagram of the studied process can be seen in Figure 1. The process is based on a similar plant operated by Exxon Mobile. The working fluid is propylene.



Figure 1: Process flow diagram of the studied process.

The process consists of two compressors in a series configuration which are driven by a single steam turbine. The compressed working fluid is condensed in the condenser using air cooling. A receiver is used as a buffer tank.

From the receiver the process stream is sent to an intermediate pressure (IP) flash evaporator. Only a small process load is removed at this stage. The fraction of gas and liquid can be adjusted by opening or closing the valves XV1 and XV2.

The saturated liquid is expanded over XV2 and evaporated in the low pressure (LP) kettle reboiler. The

main process load is removed in the kettle reboiler. The heating of the working fluid is achieved with heating coils which are submerged in the two evaporators. On the inside of the coils flows a hot process stream which is sought to be cooled down.

A detailed description of the model equations and the necessary assumptions are given in Section 3

# Part I Theory

This part contains some basic theory. It is meant to give a brief summary of the applied methods such as the steps in the top-down procedure for control structure design. It is assumed that the reader already has insight in the described theory. If the reader lacks the necessary background knowledge, it is recommended to read Skogestads paper on the subject [10] for a quick introduction. The idea behind this part is to give the reader a quick reminder of the applied theory, but it is not strictly necessary to read it in order to understand the rest of the report.

## 2 Top down procedure for control structure design

The top down procedure for control structure design is a useful tool for determining what needs to be controlled [10]. Skogestad defines four steps for the top down procedure:

#### 2.1 Defining the operational objective

The first step is to define the objective. The objective is defined as a cost function which is to be minimized, subject to a set of equality constraints and a set of inequality constraints.

$$\min_{u} J(u,d) \quad s.t \quad g_1(u,d) = 0 \quad , \quad g_2(u,d) \le 0 \tag{1}$$

Common objectives for control include maximization of throughput and minimization of energy consumption. Linear combinations of multiple objectives can also be used to find the optimal trade-off. The objectives very often relate to some kind of economic cost.

The constraints, i.e. the functions  $g_1$  and  $g_2$ , must also be defined. The limits imposed on the variables depend on the physical constraints of the equipment, product specifications etc. The model equations are included as part of the equality constraints.

#### 2.2 Degree of freedom analysis

The degrees of freedom of a system are used to control it. The number of dynamic degrees of freedom can be found by counting the number of MV's. Typically only those degrees of freedom which have a steady-state effect will have an effect on the cost. The number of steady-state degrees of freedom can be expressed as: [10]

$$N_{ss} = N_{MV} - N_0 \tag{2}$$

Where  $N_0$  are the number of dynamic degrees of freedom which have no steady-state effect. Jensen and Skogestad describe a method for finding the steady-state degrees of freedom of refrigeration cycles [7]. For a single component, the steady-state degrees of freedom equal to the number of MVs minus the number of liquid receivers exceeding the first one.

After the degrees of freedom have been found, the process can be optimized using the remaining degrees of freedom. The problem is a mathematical programming problem and is solved using numerical tools. Constraints that are on their respective limits are called active constraints. Active constraints will need to be be controlled since they have a large effect on the cost function, as can be seen from Equation (3). Equation (3) shows the truncated Taylor expansion of the cost function around the nominal point, written in terms of the independent variables.

$$J(c,d) = J^*(c,d) + \lambda \left( c_{act} - c^*_{act}(d) \right) + (c - c^*(d))^T J_{cc}(c - c^*(d))$$
(3)

In the above equation, c are the independent variables and  $c_{act}$  are active constraints.  $\lambda$  is the Lagrange multiplier. The star (\*) subscript indicates values at the nominal point. As can be seen, the cost function is

linearly correlated to the active constraints. For small disturbances, this means that the active constraints contribute more to the loss than the unconstrained variables. This means that the active constraints must be controlled.

#### 2.3 Implementation of optimal solution

The optimal solution that is found is implemented. As discussed previously, some of the degrees of freedom must be used to control the active constraints. Any remaining degrees of freedom can be used to control the process in such a way that the operation is optimal even when disturbances occur. This is called selfoptimizing control, since the loss stays acceptably low even though the process is disturbed. It would be preferable to control the gradient of the cost directly, such that  $J_u = 0$  at all times. Unfortunately this is often not possible since the gradient is difficult to measure. Instead, one chooses to control a combination of inputs such that it stays at a constant setpoint. If H is chosen correctly, this will ensure that  $J_u \approx 0$ .

$$c = Hy \tag{4}$$

Where H is called the selection matrix. There are different methods to find H:

- Brute force evaluation. Evaluate  $Loss = J(c + \epsilon_n, d) J^*(u)$ , where  $\epsilon_n$  is the implementation error, and select the variable c with the smallest loss.
- Nullspace method. Choose H such that HF = 0, where F is the sensitivity matrix defined as  $F = \frac{\partial y^*}{\partial d}$ . The nullspace method gives zero loss from optimal operation for any disturbance given that there is no implementation error, but it can only be used if there are enough measurements. The number of measurements must satisfy the inequality  $n_u + n_d \leq n_y$ . For a detailed description of the nullspace method, see Alstad and Skogestad [1].
- Exact local method. Since the nullspace method is only accurate if there is no implementation error, the exact local method was developed by Alstad et. al. [2] with roots in the exact method proposed by Halvorsen et. al. [6]. The exact local method involves minimizing the problem

$$\min_{H} ||J_{uu}^{0.5} (HG^y)^{-1} H[FW_d W_{n^y}]||_F \tag{5}$$

For information about the notation it is referred to the original paper by Alstad. Otherwise the method and the corresponding notation will be explained when used later in the report.

Alstad and Skogestad give the following criteria for the choice of self-optimizing variables

- 1. c should be insensitive to disturbances at the optimum, i.e. the optimum should not be expected to move when the process is disturbed.
- 2. The optimum should be flat to minimize the effect of implementation error. That is to say that  $J_{cc}$  should be small, i.e. that the concavity of  $J^*$  is small.
- 3. c should be easy to implement and control. This means for example that temperature and pressure measurements are preferred to composition measurements, as they are cheaper and more reliable.

#### 2.4 Production rate and inventory control

Lastly, it is necessary to choose where to set the production rate. The throughput manipulator lets the operators choose how to operate the plant. If no degrees of freedom are left, the process does not have a possibility to set the production rate. Instead, the throughput is determined by upstream process units. The location of the TPM should be chosen such that it is close to any bottlenecks in the process [3].

Gas and liquid inventories must be controlled to keep them within acceptable bounds as defined by the constraints. Aske and Skogestad defined consistent inventory control as "An inventory control system is consistent if it can achieve acceptable inventory regulation for any part of the process, including the individual units and the overall plant" [3]. In other words, the mass balance must be satisfied for the overall process and for the individual units. Local consistency adds the additional criterion that each unit must fulfil the mass balance, even when viewed separately from the process as a whole.

For a closed system, it is advised to set the TPM to one of the streams inside the loop to avoid snowballing. The snowballing effect describes the steady-state phenomenon when a small change in the feed to the system results in a large change in the recycle flow rate [9]. This effect can be avoided by moving the TPM inside the recycle loop. It is also necessary to leave one of the inventories inside the loop uncontrolled. Not doing so will overspecify the system and violate the consistency rules [3].

# Part II Results

# 3 Modelling

The necessary equations and correlations for modelling the process were found in Chapter 3 of Asmar's thesis [4]. A complete description of the model can be found there. The core assumptions done in the modelling can be summarized as follows:

- Compressors are modelled based on compressor curves for existing equipment. This means that the model must be rewritten if applied to a different system.
- The coils in the evaporators are fully submerged at all times. The heat transfer coefficient for the heat transfer between the working fluid and the hot process streams is assumed to be independent of temperature. A constant value for *UA* is thus used. It is also assumed that there is no heat loss through the walls of the equipment.
- The process streams are modelled as single-phase streams. Their thermodynamic properties such as heat capacity are assumed to be constant on the given temperature interval.
- The thermodynamic properties of propylene are approximated as linear functions of the temperature over the studied temperature interval. The relationship between the saturation pressure and temperature is given by the Antoine equation.
- The process equipment has no capacity and does not undergo thermal expansion.
- The levels are assumed to be linearly correlated to the volumetric liquid hold-ups in the tanks. This assumption fails if the cross-sectional area of the tank is not constant.
- Propylene expands adiabatically over expansion valves. This results in a pressure and temperature drop, as heat is removed from the working fluid to form flash-vapour.

The system contains a number of implicit variables such as the temperatures. The system can be written as a combination of differential and algebraic equations. DAE-systems of this kind are solved in MATLAB with the built-in ode15s procedure.

Inspection shows that the system has 5 degrees of freedom. These 5 degrees of freedom are represented as control valves in Figure 1. XV1, XV2 and XV3 are valve openings, whereas N is to the rotational speed of the steam turbine and FCP3 corresponds to the heat removed from the condenser.

### 3.1 Model equations

The following sections describe the system of equations that has to be solved, in detail. The model equations will be presented in a logical order, though the final model does not depict this.

All model equations are taken from Asmar [4]. They are repeated here for reader convenience. Asmar describes a general system consisting of n compression stages. The notation has been kept even though this report considers a process consisting of only two evaporators and two compressors.

All parameters that are used in the equations are summarized in Appendix A.

#### 3.1.1 Evaporators



Figure 2: Illustration of an evaporator.

The mass balance for the evaporator shown in Figure 2 can be written as

$$\frac{dW_i}{dt} = FL_{i+1} - FL_i - FG_i \tag{6}$$

where FL are the liquid flows in and out of the evaporator and FG is the gas flow rate of the evaporator. This gives the change in refrigerant hold-up W in the evaporator. From the hold-up W, the level can be calculated indirectly. Assuming that the cross-sectional area of the evaporator is constant, i.e. that the evaporator is cylindrically-shaped, then the level of the refrigerant is proportional to the volumetric liquid hold-up, WLV.

$$L_i \propto W L V_i \tag{7}$$

The volumetric liquid hold-up can be calculated as

$$WLV_i = WL_i \cdot v_{f,i} \tag{8}$$

Where  $v_f$  is the liquid specific volume of propylene. The specific volume is assumed to be a linear function of temperature, and can thus be calculated as

$$v_{f,i} = \lambda_1 + \lambda_2 \cdot T_i \tag{9}$$

where  $\lambda_i$  are constant coefficients which are determined experimentally. The values for the coefficients are given in Table 8 in the Appendix.

The liquid hold-up WL can not be calculated directly, but must instead be calculated iteratively from the mass balance over the vessel inventory

$$W_i = WL_i + WV_i \tag{10}$$

Flow rates are determined by the fractional valve openings of the control valves. The flows are assumed to be proportional to the square root of the pressure drop over the valve.

$$FL_{i+1} = XVL_i \cdot CVL_i \sqrt{\Delta P} \tag{11}$$

In the above equation, XVL is the fractional value opening and CVL is a constant coefficient. The same equation is used for calculating the vapour flow rates.

$$FG_i = XVG_i \cdot CVG_i \sqrt{\Delta P} \tag{12}$$

For the first evaporator, there is no valve on the vapour outlet, such that the flow rate solely depends on the suction pressure of the compressor.

The pressure in the evaporator is the saturation pressure  $P_i$ , which is a function of the temperature. Antoine's equation is used to calculate the saturation pressure as a function of temperature.

$$P_i = \exp\left(A - \frac{B}{T_i - C}\right) \tag{13}$$

In the above equation, A, B and C are constants. The values of the constants are given in Table 3 in the Appendix. The saturation temperature  $T_i$  must be calculated from the energy balance. Since the energy balance cannot be solved explicitly for the temperature, it must be calculated iteratively.

$$H_i = WL_i \cdot HFL_i + WV_i \cdot HFG_i \tag{14}$$

The dynamic energy balance for the evaporator can be written as

$$\frac{dH_i}{dt} = (HFL \cdot FL)_{i+1} - (HFL \cdot FL)_i - (HFG \cdot FG)_i + Q_i \tag{15}$$

where HFL is the specific enthalpy of the liquid stream and HFG is the specific enthalpy of the gas stream.  $Q_i$  is the heat transferred from the process stream inside the heating coils to the refrigerant in the vessel. The specific enthalpies are assumed to be linear functions of the temperature

$$HFG_i = \zeta_1 + \zeta_2 \cdot T_i \tag{16}$$

$$HFL_i = \delta_1 + \delta_2 \cdot T_i \tag{17}$$

The heat load  $Q_i$  is specified through the temperatures of the process stream in and out of the evaporator, in addition to the process stream mass flow rate. These parameters are either specified or used as disturbances in the calculations.

$$Q_i = FCP_i \left(TP_i i - TP_i o\right) \tag{18}$$

$$TP_i o = (1 - \alpha_i) T_{i+1} + \alpha_i TP_i i \tag{19}$$

where

$$\alpha_i = \exp\left(\frac{-U_i \cdot A_i}{FCP_i}\right) \tag{20}$$

U and A are the heat transfer coefficient and the heat transfer area, respectively. FCP is the product of the heat capacity and the flowrate of the process stream.

#### 3.1.2 Condenser and receiver



Figure 3: Illustration of the condenser and receiver

After the vapour refrigerant exits the second compressor, it enters the condenser with pressure equal to the discharge pressure of the compressor. The refrigerant exchanges heat with cold air and condenses. The temperature is calculated using the Antoine equation. Condensed refrigerant is stored inside the receiver, as it is assumed that no liquid refrigerant remains in the condenser. The mass balance over the condenser can thus be written as

$$\frac{dWV_c}{dt} = FGCD_n - FL_c \tag{21}$$

The total vapour hold-up can be calculated by summation of the vapour contained in the receiver and the vapour contained in the condenser. Since the condenser does not contain any liquid, the vapour hold-up in the condenser equals to the total condenser volume.

$$VG_c = V_c + V_r - (WL_r \cdot v_{f,r}) \tag{22}$$

The receiver liquid hold up  $WL_r$  is calculated from a total balance over all inventories in the system.

$$WL_r = W - \sum_{i}^{n} W_i - WV_c \tag{23}$$

For this system n = 2, meaning that the total mass in the system equals to the masses contained in the two evaporators plus the mass contained in the condenser and the receiver. It can be shown that the energy balance simplifies to

$$\frac{dT_r}{dt} = \frac{FL_c}{WL_r} \left( T_c - T_r \right) \tag{24}$$

In the above expression, the liquid refrigerant flow rate from the condenser,  $FL_c$ , can be calculated as

$$FL_c = \frac{Q_c}{HFG_c - HFL_c} \tag{25}$$

The specific enthalpies of the gas phase and the liquid phase are calculated using Equations (16) and (17) with the corresponding condenser temperature.  $Q_c$  is calculated the same way as for the two evaporators, using Equations (18), (19) and (20).

#### 3.1.3 Compressor



Figure 4: Illustration of a generic compressor stage. Notice that the figure must be modified for the first compression stage, as it does not have interstage mixing.

The suction mass flowrate into the compressor is given by

$$FGCS_i = FGV_i \frac{M_w \cdot PS_i}{TS_i \cdot R \cdot z_i} \tag{26}$$

This is the equation of state where TS and PS are the suction temperature and pressure, z is the compressability factor and FGV is the inlet volumetric vapour flowrate of refrigerant.  $M_w$  is the molecular weight of propylene and R is the universal gas constant. The compressability factor z is approximated as a linear function of the temperature

$$z = \phi_1 + \phi_2 \cdot T \tag{27}$$

As can be seen from Figure 4, the suction mass flowrate entering the compressor generally must satisfy the following mass balance

$$FGCS_i = FGCD_{i+1} + FG_i \tag{28}$$

where FGCD is the discharge mass flow rate from the previous compressor and FG is the vapour flow rate from the corresponding evaporator. Equation (28) does not apply to the first compressor stage, as there is no interstage mixing.

The interstage mixing temperature TS is calculated from the energy balance.

$$TS_i = \frac{TD_{i-1} \cdot FGCD_{i-1} + T_i \cdot FG_i}{FGCD_{i-1} + FG_i}$$
(29)

The compressor equations are based on compressor curves. These are curves relating to the performance of the compressor which are found from experimental data.

$$\frac{FGV_i}{N^q} = f_i(hs_i) \tag{30}$$

In the above expression, N is the fractional compressor speed, q is a constant and f is the compressor curve. Each compressor has a unique compressor curve and q-value. hs is the scaled compressor head, and is defined as

$$hs_i = \frac{h_i}{N^p} \tag{31}$$

p is a constant value depending on the compressor.

For polytropic compression, the compression head can be expressed as

$$h_i = k_i \frac{R}{g \cdot M_w} \left( TD_i - TS_i \right) \tag{32}$$

g is the gravitational constant. The discharge temperature can be calculated as

$$TD_i = \frac{TS_i}{\left(\frac{PD_i}{PS_i}\right)^{\frac{1}{k_i}}} \tag{33}$$

 $k_i$  is a constant value which is defined as

$$k_i = \frac{n}{n-1} = \frac{\eta \gamma_{avg,i}}{\gamma_{avg,i} - 1} \tag{34}$$

In the above expression, n is the polytropic exponent and  $\nu$  is the polytropic efficiency of the compressor, which is given by

$$\eta_i = f 2_i (h s_i) \tag{35}$$

Similarly to the compressor curve f, f2 is found by fitting experimental data from a specific compressor unit. Finally,  $\gamma_{avg}$  is the averaged ratios between the specific heats (adiabatic ratios) between suction and discharge.

$$\gamma_{avg} = \frac{1}{2} \left( \frac{CPI_i}{CPI_i - R} + \frac{CPO_i}{CPO_i - R} \right)$$
(36)

CPI is the heat capacity at inlet (suction) conditions, whereas CPO is the heat capacity at outlet (discharge) conditions. The heat capacities are approximated as fifth order polynomials of the temperature.

$$CP = C_1 + C_2 \cdot T \left( C_3 + C_4 \cdot T \left( C_5 + C_6 \cdot T \right) \right)$$
(37)

The values of the coefficients in Equation (37) are given in Table 4 in the Appendix.

By fitting data from the supplier to the performance of the compressors, the compressor curve for the first compressor was found to be

$$f_1(hs_1) = \frac{FGV_1}{N^q} = \frac{C_{11} \cdot hs_1 - C_{12}}{C_{13}}$$
(38)

For the second compressor

$$f_2(hs_2) = \frac{FGV_2}{N^q} = C_{24} + C_{25}\log\left(\left(\sqrt{TX^2 + 1}\right) - TX\right)$$
(39)

TX is defined as

$$TX = \frac{C_{21}}{\tan\left(\frac{C_{22} - hs_2}{C_{23}}\right)}$$
(40)

The parameters for Equation (38) can be seen in Table 9 in the Appendix. The parameters for Equation (39) can be seen in Table 10 in the Appendix.

In a similar fashion, f2 is found by fitting actual performance data. For both compressors, the following relationship can be used

$$\eta_i = f2_i(hs_i) = e_1 \cdot hs_i + e_2 - 10^{(e_3 \cdot hs_i - e_4)} \tag{41}$$

The parameters for Equation (41) can be seen in Table 11 in the Appendix.

#### **3.2** Implementation in MATLAB

The original model by Asmar is written in ACSL and had to be translated to MATLAB. The differences between the original script by Asmar and the script that was implemented in MATLAB were mainly a result of the differences between the programming languages. Though the actual model equations stayed the same, the rest of the script had to be rewritten to work in MATLAB. ACSL is structured very unlike MATLAB. First, all variables are initialised and initial estimates are assigned to them. The equations are then stated as algebraic or differential equations and integrated directly through a call to the INTEG-function. The order of the equations does not seem to be of importance, so that variables can be used before values have assigned to them. In MATLAB it is necessary to define the set of equations in chronological order and then call an integrator such as ode15s from a different script to integrate the equation system.

The resulting MATLAB-code can be seen in Appendix **REF** 

### 4 Dynamic simulation

In this section, the dynamic behaviour of the developed model is described. Though the focus of this report is not primarily to study the dynamic behaviour of the model, it is necessary to do so in order to find out which variables need to be controlled in the stabilizing layer of the control structure, i.e. finding variables which are not self-regulatory [8]

#### 4.1 Controlling the levels

It was attempted to find a steady state solution of the equation system, i.e. solving the following equation

$$f(\mathbf{x}) = \begin{bmatrix} f_{\text{diff}} \\ f_{\text{alg}} \end{bmatrix} = \mathbf{0}$$
(42)

$$f_{\text{diff}} = \frac{\partial g(\mathbf{x})}{\partial t} \tag{43}$$

However, simulations revealed that the levels were not self-regulatory, and that they would integrate to positive or negative infinity. A fairly constant level is desired to make sure that the coils in the evaporators are submerged at all times. It was therefore decided to implement controllers before attempting to optimize the system. P-controllers were chosen because of their ease of implementation. The resulting setpoint offset can be accepted because there is no need to control the levels tightly.

In correspondence with the rules on consistent inventory control proposed by Aske and Skogestad [3] one of the inventories was left uncontrolled. This was done to avoid over-specification of the mass streams in the closed system. It was chosen to control the levels of the two evaporators,  $L_1$  and  $L_2$ , and leave the level of the receiver,  $L_3$ , uncontrolled. The uncontrolled inventory will be indirectly controlled when all the other inventories are controlled (the total mass in the system is conserved), but the control will be slow due to the large time delay. This large time delay will cause large variations in the level. Since the receiver is the largest inventory in the loop, it is best suited to deal with level variations. The two smaller inventories have smaller tolerances for level variations, and thus require tighter level control. An illustration of the proposed control structure can be seen in Figure 5



Figure 5: Process flow diagram of the studied process with the two added level control structures.

The selection of MV's for controlling the two levels was based on intuition and general pairing rules. XV2 was paired with  $L_1$  since it has the most direct effect. XV3 could also have been chosen, but this would have lead to local inconsistency [3] and is a violation of the "pair close" tuning rule. After closing the first level control loop, XV3 and XV1 are the only remaining CV's having a direct effect on the  $L_2$ . Both fulfill the "pair close"-rule, but since XV3 has a more direct effect on the level,  $L_2$  was paired with XV3.

The controllers were tuned by trail and error. It was found that a  $K_c$ -value of 0.5 gave satisfactory disturbance rejection without causing the controllers to saturate.

#### 4.2 Dynamic responses

After the liquid inventories were controlled, the dynamic performance of the model was tested. The responses to a setpoint change in L1 are seen in Figure 6. A disturbance in TP1I was also simulated. The results of the simulation can be seen in Figure 7.

The responses seem okay at first glance. A more in-debt analysis of the results can be found in the discussion



in Section 7.1. The main focus of this project is the steady-state behaviour of the model, and the rest of the report will deal with the steady-state behaviour of the model unless something else is stated.

Figure 6: Dynamic responses for some selected variables for a 10% increase in the setpoint of L1



Figure 7: Dynamic responses for some selected variables for a 5% increase in TP1I.

## 5 Steady-state optimization

This section describes how the optimal operating conditions were found.

### 5.1 Determining the steady-state effect of the levels

At first the author ran the optimization with the setpoints for the level controllers being two optimizable degrees of freedom. The optimization showed that the setpoints influenced the total energy consumption. However, closer inspection showed that this behaviour was caused by numerical instability and that the cost function was not influenced by the levels after all. Figure 8 shows the optimal value of the cost function J as a function of the setpoints for L2 and L1. The cost function is more or less constant for all combinations of L2 and L1, except when both setpoints go towards their minimum values. Most likely this is a result of the optimizer not being able to find a solution that satisfies the constraints, and thus stalling prematurely. The figure also shows a small 'trench' for L1 approximately equal to 3.7. It is not known what causes this, but it is likely to be attributed to numerics and not represent an actual steady-state effect of the level setpoints.



Figure 8: Optimal value of cost function J with fixed values for the setpoints of L1 and L2

Though levels can have a steady-state effect, as is the case for non-equilibrium liquid phase reactors [8], they do not effect the steady state in this case. The opposite would have been true if the heat-transfer in the cooling coils would have depended on the liquid level in the tank, but this effect is not included in the model.

The two level-controllers remove two steady-state degrees of freedom, so that the remaining steady-state

degrees of freedom is reduced to three. This follows from Equation (2). The same result can be found by applying the method to find steady-state degrees of freedom of refrigeration cycles described by Jensen and Skogestad.

### 5.2 Nominal operating conditions

The nominal operating conditions can be found by minimizing a nonlinear mathematical programming problem. The cost function that is to be minimized is the total energy consumption of the two compressors. Constraints were introduced to keep the variables within a reasonable operating ranges. In chapter 5 of Asmar's thesis[4], the ranges for some of the process variables are given. The constraints for the measured variables and the inputs are given in Table 1 and Table 2, respectively.

Table 1: Ranges for the measured variables, taken from [4]. Notice that the unit for the levels is  $m^3$ . This is because the volumetric liquid hold-up is controlled rather than the level.

Variable	$\begin{array}{c} L_1 \\ [\mathrm{m}^3] \end{array}$	$L_2$ [m <sup>3</sup> ]	$L_3$ [m <sup>3</sup> ]	$P_1$ [bar]	$P_2$ [bar]	$P_3$ [bar]	$\begin{array}{c} T_{P,1,o} \\ [\mathrm{K}] \end{array}$	$F_{L,2}$ [kg/s]	$F_{L,3}$ [kg/s]	$\frac{F_{G,2}}{[kg/s]}$
Lower boundary Upper boundary	$2.9 \\ 6.4$	$0.6 \\ 1.6$	$6.9 \\ 13.7$	$\begin{array}{c} 0 \\ 2 \end{array}$	$\frac{3}{6}$	12 18	$\begin{array}{c} 200\\ 300 \end{array}$	$\begin{array}{c} 0 \\ 5.47 \end{array}$	0 7.18	$\begin{array}{c} 0 \\ 6.31 \end{array}$

Variable	XV1 [-]	XV2 [-]	XV3 [-]	N [-]	$\begin{array}{c} FCP3 \\ [\frac{J}{s\ K}] \end{array}$
Lower boundary Upper boundary	$\begin{array}{c} 0 \\ 1 \end{array}$	$\begin{array}{c} 0 \\ 1 \end{array}$	$\begin{array}{c} 0 \\ 1 \end{array}$	$\begin{array}{c} 0.9 \\ 1.1 \end{array}$	$\frac{116}{348}$

Table 2: Ranges for the input variables, taken from [4]

Other, unconstrained state variables were specified to lie within the range zero to infinity. In addition to the constraints on the inputs and the state variables, the optimizer needs a set of equality and inequality constraints. The DAE-system was provided as an equality constraint, meaning that the steady-state optimal conditions are found. The setpoints for the levels were also set as equality constraints. The maximum allowable outflow temperatures of the process streams from the evaporators were specified as inequality constraints.

In addition to the specified constraints for the variables, one must also specify the load of the refrigeration cycle, otherwise the optimizer will attempt to shut down the process by letting N and FCP3 go to their lower limits. XV1 was approaching its lower limit, but the upper pressure constraint for P2 was reached before this happened. Relaxing the pressure constraint led to XV1 fully closing. The load was specified as inequality constraints for the outflow temperatures of the process streams from the evaporators. TP2O is required to lower than or equal to 276.75°C. The upper limit of TP1O is set to 226.20°C. These values were found in Appendix A of Asmar's thesis [4]

Figure 5.2 shows the calculated optimum given the set of constraints previously mentioned. It can be noted that FCP3 is at its upper limit, making it an active constraint. Both constrained process outflow temperatures, TP2O and TP1O, are at their upper allowable limits. This is to be expected, since lowering their temperatures would lead to higher energy consumption. These constraints are thus also active. All active constraints are coloured red in Figure 5.2. The cost function evaluates to an energy consumption of  $7.989 \cdot 10^5$  W.



### 5.3 Self-optimizing control

It was originally planned to find a self-optimizing control structure for the process. However, this requires unconstrained degrees of freedom. The results from the optimization show that three constraints are active at the nominal point. This leaves zero unconstrained degrees of freedom left which can be used for selfoptimizing control. In other words, the process is constrained in such a way that only one solution is possible at the optimal operating point.

# 6 Alternative process layout

In an attempt to free one degree of freedom in the system, it was suggested that one could connect the process streams such that the outflow from the second evaporator becomes the inflow of the first evaporator. The idea behind this is to decrease the number of independent heat load specifications from two to one. The cost function was also changed such that the objective was to maximise heat transfer rather than minimizing the energy consumption. It was thought that this would give an additional degree of freedom being the distribution of transferred heat between the two evaporators. The proposed process layout can be seen in Figure 9

Since the heat transfer is very different in the two evaporators, it was not possible to just connect them without adjusting the parameters. This proved to be a non-trivial task, as the optimizer struggled to find a solution of the updated process. The flow rates of the two process streams were combined to give the new flow rate of the process stream. The product of the heat transfer areas and the heat transfer coefficients, UA, were difficult to adjust. Hereafter, UA will be referred to simply as the heat transfer area. This makes logical sense because the heat transfer coefficient is expected to remain relatively constant, while the area can be moved from one evaporator to the other. It should be mentioned that the distribution of area is a question of design optimization and not control optimization. As such, it does not really concern this project. However, since the alternative case needs to have properly defined parameters, it will be explored how changing the design could lead to a less or more interesting case.

It was attempted to move heat transfer area from one evaporator to the other while keeping the overall area constant. This led to problems as the optimizer would not find a solution. Initial conditions were either badly defined or the system was set up in such a way that no solution existed. It was observed that the optimizer was able to find a solution if both heat transfer areas were reduced to about 30 W/K. It was also noticed that small changes in the distribution of the areas led to a change in the active constraints. In order to find the active constraint regions, the system was optimized for a range of areas around 30 W/K. The



Figure 9: Process flow diagram of the considered alternative process.

resulting active constraint regions can be seen in Figure 10. The corresponding cost function can be seen in Figure 11  $\,$ 

Eight main constraint regions are observed. The active constraints in each region are, beginning on the top, going clockwise:

- Region 1 (grey): XV1, FCP3 and XV2.
- Region 2 (dark blue): XV1, XV2 and XV3.
- Region 3 (red): XV1, XV3 and P3.
- Region 4 (purple): N, XV1 and XV3.
- Region 5 (orange): N, XV1 and FCP3.
- Region 6 (blue): N, FCP3 and XV2.
- Region 7 (pink): N, XV2 and XV3.
- Region 8 (green): XV2.

All the constraints are active and at their upper limits. There are some other constraint regions as well, but these regions are very small. A total of 21 regions were found.



Figure 10: Active constraint regions for different combinations of the heat transfer areas in the two evaporators.

Figure 11: Cost as a function of the heat transfer areas U1A1 and U2A2.

Since there are three active constraints in all regions except for region eight, it is not possible to implement a self-optimizing control structure for most combinations of U1A1 and U2A2. It would be theoretically possible to implement self-optimizing control in region eight since there is only one constrained degree of freedom

in this region. That leaves two unconstrained degrees of freedom for optimization. It is also observed that the border between region two and region three gives the lowest possible value of the cost function for the studied intervals of U1A1 and U2A2. Which region it is best to be in will be discussed in greater detail in the discussion in Section 7

# Part III Discussion, conclusion and suggestions for further work

# 7 Discussion of the results

This section tries to explain the results from Part II.

### 7.1 Dynamic responses

The dynamic behaviour of the developed model is described in Section 4. Since the levels were not self-regulatory, they had to be controlled. As can be seen from Figure 6 and Figure 7, the levels are now controlled. The responses are relatively slow, as L1 seems to have a closed-loop time constant of about 250 seconds. This response can be attributed to the poor tuning of the controller. The P-controller was not tuned systematically. Instead, a Kc value was chosen such that the controller would not saturate given a reasonable (10%) disturbance. Faster control can be achieved by tuning the controller more aggressively, though this might lead to saturation. It is also observed that L2 reacts quite slowly to a setpoint change in L1 due to delay. This can be avoided by implementing a cascade or feed-forward controller. However, this was not deemed necessary. Finally, it is observed that L3 is as slow as the slowest of the two other levels. This is because it is not controlled directly.

From Figure 6 it can be seen that there is a steady-state offset for L1. As the setpoint for the level is increased by 10% from 3.1 to 3.41, the actual steady-state value of L1 is closer to 3.5. The offset is due to the lack of integral action, since the levels are controlled by pure P-controllers. It can also be seen that the response of T3 is very slow. This is probably due to the large capacity of the system and the transport delay.

Figure 7 shows the dynamic responses to a disturbance in TP1I. The 5% increase in TP1I leads to a larger amount of heat transferred to the refrigerant, which causes more refrigerant to evaporate. This leads to the observed drop of the level in the first evaporator. The level controller reacts by opening XV2, which causes the level in the second evaporator to drop as well. L3 follows after a little delay. T1 rises due to the increased heat transfer. T2 follows quite quickly due to the pressure equilibrium that is established in the saturated refrigerant. T3 increases much more slowly due to the large capacity of the tank. It takes much more time to heat up the large hold-up of refrigerant in the receiver. The hold-up of liquid in the receiver is more than eight times larger than that of the second evaporator, so it makes sense that the temperature increases much more slowly. The increased pressure spreads almost immediately from P1 to P3 to P2, as is to be expected.

Overall, the dynamic responses seem to correspond well with what is expected from intuition and theory. It is therefore safe to assume that the implemented model gives a reasonable approximation of the actual process.

### 7.2 Steady-state optimization

As already discussed, it is expected that the setpoints for the levels do not have a steady-state effect based on literature. A brute-force evaluation of the cost function for different setpoints shows the same result. With the exception of when both setpoints were close to their lower boundaries, the cost function is approximately constant. The observed deviations for small values of L1 and L2 were most likely due to violations of the upper constraint for L3. The border between the stable region and the unstable region seems to follow a linear relationship, which strengthens this theory. The border line represents the case where the upper constraint for L3 is active. The linearity of the border follows directly from the mass balance.

At the nominal operating point it was found that both the upper temperature specifications for the process

outflows were active. This makes sense, as the objective was to minimize the energy consumption. Cooling the process streams more than necessary would be a give-away of energy and thus increase the cost. Since both heat loads can be specified independently, it is possible to have both active. In addition, it was observed that the condenser duty is maximised by letting the flow of air being at its upper constraint. This is to be expected since more cooling leads to a lower pressure and a lower temperature in the evaporators, allowing for more cooling. Since there is no cost associated with the condenser, this constraint will always be active when trying to minimize the energy consumption.

When no heat load was specified, it was observed that N went to its lower boundary. This is to be expected, since the optimizer tries to minimize the energy consumption by shutting of the compressor train. FCP3 also went to its lower boundary to avoid pressure drop which would cost unnecessary energy loss in the compressor train. P2 was at its upper boundary since the valve XV2 was trying to close completely to avoid bypass of gas. By closing XV2 it can be made sure that all the gas goes through both compressors, thus utilizing the energy as efficiently as possible.

Based on these two cases, it seems that the optimizer was set up properly and that the model gives reasonable results.

### 7.3 Alternative process layout

The alternative case was defined in order to free some degrees of freedom by combining the two heat load specifications to one. It was hoped that this would open up a degree of freedom being the distribution of liquid in the two tanks, i.e. how much cooling is done in each of the evaporators.

Problems arose when trying to find fitting parameters for the new model. The distribution of heat transfer areas area in the two evaporators caused trouble as it was not possible to distribute the old heat transfer areas equally between the two evaporators. A solution was found when U1A1 was set equal to approximately 30 W/K. However, the active constraints are very sensitive to the exact distribution of area, as can be seen in Figure 10. A total of 21 different constraint combinations were observed, though most of them only existed in a single point or in very small regions. It is therefore relatively safe to assume that the eight main regions are the correct ones, whereas the smaller ones were caused by numerical error or strange model behaviour on the border between two constraint regions.

All except for one of the main constraint regions have three active constraint. Region eight is the exception with only one active constraint. It is theoretically possible to implement self-optimizing control in this region, but this might not be the best overall solution. As can be seen from Figure 11, the total heat transfer is larger in region two and three. Whether or not it is better to stay in region eight depends on the sensitivity of the cost function there. It would be preferable to have a flat cost function curve at this point [8][5] In addition, it is desirable that changes in the inputs do not cause any constraints to become active, as that would make control very difficult as some sort of event detection would be needed to switch between different control structures. The desire for a flat optimum obviously goes for all constraint regions. The sensitivity has not yet been found, so it is difficult to say which of these eight regions would be the best choice for implementation.

It is worthwhile to notice that the attempt to gain additional degrees of freedom by connecting the two evaporators, failed. There are still three active constraints and zero unconstrained degrees of freedom in the system, with the exception of the previously mentioned region eight. It is hard to spot a reason for why the active regions are placed where they are, but it could seem as if the optimizer tries to maximise the heat transfer in the most effective evaporator first and then maximise the other one if possible. This means that the distribution of heat in the two evaporators does not give a degree of freedom as previously assumed. However, this is just a very early hypothesis that needs more investigation to be verified.

It should also be mentioned at this point that while the above discussion assumes that the distribution of heat transfer area can be chosen freely to optimize the operation, this is generally not possible. The plant has predetermined equipment that needs to be operated as optimal as possible, even though the plant might run more efficiently if the process layout was changed. It is not the objective of the control engineer to change the layout of the plant, but rather to operate the existing plant to the best of its abilities. But the determination of the constraint regions is not completely useless from a control point of view. Once the design has been finalized and the plant has been built, the process can still go from one constraint region to another. Fouling inside the evaporator can lead to a decrease in the heat transfer coefficient, thus lowering the UA-value. If the plant is designed in such a way that it operates in region three, for example, it is very likely that it switches from region three to region two or four over time due to fouling. This knowledge will be valuable to the operators of the plant.

# 8 Conclusion

A model for a two-stage refrigeration cycle was implemented in MATLAB. Dynamic simulations were done to verify the model. The model was optimized at steady state and the nominal operating point was found. Degree of freedom analysis showed that not enough unconstrained degrees of freedom were left to implement self-optimizing control. An alternative case was created to get more degrees of freedom. Finding the optimal parameters for the new models is non-trivial, since a large amount of active constraint regions are present. One of the constraint regions only contains one active constraint, so it would be possible to implement a self-optimizing control structure in this region. This was not done due to time restrictions.

## 9 Suggestions for further work

- Look at the alternative case in depth. Determine what region is most realistic or interesting to study.
- Exxon suggested that one should let the differences TP1I-T1 and TP2I-T2 be constant instead of TP1I and TP2I. The cost function should be changed to include a trade-off between the energy consumption and the recovery of high-value molecules as indicated by the heat transfer in the evaporators.
- Dynamic optimization / MPC

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# Appendices

## A Parameters used for the simulations

In the following tables, the coefficients for the model equations will be given. All values were taken from Asmar [4]

Table 3: Coefficients for the	Antoine equation	in Equation (	(13)	)
-------------------------------	------------------	---------------	------	---

Variable	A	В	C	
	[-]	[-]	[-]	
Value	9.0825	1807.53	26.15	

Table 4: Coefficients for calculating the heat capacity of propylene in Equation (37). Calculated heat capacity has units J/(kgK)

Variable	$C_1$	$C_2$	$C_3$	$C_4$	$C_5$	$C_6$
Value	3.707	0.01	23.439	0.001	-11.594	$2.2033 \cdot 10^{-3}$

Table 5: Coefficients for calculating the compressibility of propylene as a function of temperature in Equation (27)

Variable	$\phi_1$	$\phi_2$
	[-]	$[{\rm K}^{-1}]$
Low pressure	0.995	0
Intermediate pressure	0.566	$1.26\cdot 10^{-3}$
High pressure	$2.97\cdot 10^{-3}$	-0.194

Table 6: Coefficients for calculating the specific vapour enthalpy of propylene as a function of temperature in Equation (16)

Variable	$\zeta_1 \ [{ m J/kg}]$	$\zeta_2$ [J/kgK]
Low pressure Intermediate pressure High pressure	$747.441 \\ 663.375 \\ 474.0188$	$\begin{array}{c} 1.36908 \\ 1.63599 \\ 2.09759 \end{array}$

Table 7: Coefficients for calculating the specific liquid enthalpy of propylene as a function of temperature in Equation (17)

Variable	$\delta_1$ [J/kg]	$\delta_2$ [J/kgK]
Low pressure	7.16036	2.63768
Intermediate pressure	7.16036	2.63768
High pressure	95.5601	2.32367

Variable	$\lambda_1$	$\lambda_2$
	[J/kg]	$[\mathrm{J/kgK}]$
Low pressure	$8.05418 \cdot 10^{-4}$	$3.934\cdot 10^{-6}$
Intermediate pressure	$5.91479 \cdot 10^{-4}$	$4.777 \cdot 10^{-6}$
High pressure	$7.493 \cdot 10^{-6}$	$-2.00589 \cdot 10^{-4}$

 Table 8: Coefficients for calculating the specific volume of propylene as a function of temperature in Equation (9)

Table 9: Coefficients for the compressor curve for the first compressor in Equation (38)

Variable	$\begin{array}{c} C_{11} \\ [\mathrm{m}^3/\mathrm{s}] \end{array}$	$\begin{array}{c} C_{12} \\ [\mathrm{m}^4/\mathrm{s}] \end{array}$	$\begin{array}{c} C_{13} \\ [m] \end{array}$
Value	1.9928	16791	8756.4

Table 10: Coefficients for the compressor curve for the second compressor in Equation (39) and Equation (40)

Variable	$C_{21}$ [-]	$\begin{array}{c} C_{22} \\ [m] \end{array}$	$\begin{array}{c} C_{23} \\ [m] \end{array}$	$\begin{array}{c} C_{24} \\ [\mathrm{m}^3/\mathrm{s}] \end{array}$	$\begin{array}{c} C_{25} \\ [\mathrm{m^3/s}] \end{array}$
Value	0.45615	10296	2956.2	0.816051	0.27585

Table 11: Coefficients for the compressor curves for both compressors in Equation (41)

Variable	$e_1$	$e_2$	$e_3$	$e_4$
	$[m^{-1}]$	[-]	$[m^{-1}]$	[-]
Compressor 1	$6.47\cdot 10^{-5}$	0.353	$7.101\cdot10^{-4}$	6.5963
Compressor $2$	$4.098\cdot10^{-5}$	0.364	$11.218 \cdot 10^{-4}$	12.445

## **B** MATLAB-code

This section contains the MATLAB-code which was used to calculate all the results. Only the model for the first case is included, as the alternative case is almost identical with the exception of some minor changes to the parameter initialisation, a new cost function and a new model equation being the condition that the inlet to the first evaporator is the outlet from the second evaporator.

### B.1 Model equations

DAE-system which is to be integrated.

```
function out = model(t,x,u,params)
1
2
     % Description
з
4
     %% Extracting states:
5
     H1 = x(1); % Diff.
6
     H2 = x(2); \% Diff.
7
        = x( 3); % Diff.
     T3
8
        = x(4); \% Diff.
     W1
9
        = x(5); % Diff.
     W2
10
     W4
        = x(6); \% Diff.
11
12
         = x(7); % Alg.
     T1
13
     T2
        = x(8); % Alg.
14
     PA = x(9); \% Alg.
15
     TA = x(10); % Alg.
16
     TC = x(11); % Alg.
17
     TD = x(12); \% Alg.
18
     HH1 = x(13); % Alg.
19
     HH2 = x(14); \% Alg.
20
     WV1 = x(15); \% Alg.
^{21}
     WV2 = x(16); % Alg.
22
23
     XV2 = x(17); \% Controller
^{24}
     XV3 = x(18); % Controller
25
26
     L1dummy
                = x(19); % Dummy
27
     L2dummv
                = x(20); % Dummy
28
     L3dummy
                = x(21); % Dummy
29
     P1dummy
                = x(22); % Dummy
30
     P2dummy
                = x(23); % Dummy
31
     P3dummy
                = x(24); % Dummy
32
     TP10dummy = x(25); % Dummy
33
     TP2Odummy = x(26); % Dummy
34
     TP30dummy = x(27); % Dummy
35
     FG1dummy = x(28); % Dummy
36
     FG2dummy = x(29); \% Dummy
37
     FG3dummy = x(30); % Dummy
38
     FL2dummy = x(31); \% Dummy
39
     FL3dummy = x(32); % Dummy
40
     FL4dummy
               = x(33); % Dummy
41
               = x(34); % Dummy
     TBdummy
^{42}
43
     %% Extracting inputs and disturbances
44
```

```
45
     L1sp = u(1);
46
     L2sp = u(2);
47
        = u(3);
     Ν
^{48}
     XV1 = u(4);
49
     FCP3 = u(5);
50
51
     %% Defining parameters
52
53
     if ~exist('params','var')
54
         params = init_params();
55
     end
56
57
     W = params.W;
58
     V1 = params.V1;
59
     V2 = params.V2;
60
     V3 = params.V3;
61
     VC = params.VC;
62
     C11 = params.C11;
63
     C12 = params.C12;
64
     C13 = params.C13;
65
     C21 = params.C21;
66
     C22 = params.C22;
67
     C23 = params.C23;
68
     C24 = params.C24;
69
     C25 = params.C25;
70
     E11 = params.E11;
71
     E12 = params.E12;
72
     E13 = params.E13;
73
     E14 = params.E14;
74
75
     E21 = params.E21;
     E22 = params.E22;
76
     E23 = params.E23;
77
     E24 = params.E24;
78
     U1A1 = params.U1A1;
79
     U2A2 = params.U2A2;
80
     U3A3 = params.U3A3;
81
     CV1 = params.CV1;
82
     CV2 = params.CV2;
83
     CV3 = params.CV3;
84
     FCP1 = params.FCP1;
85
     FCP2 = params.FCP2;
86
     TP1I = params.TP1I;
87
     TP2I = params.TP2I;
88
     TP3I = params.TP3I;
89
     A = params.A;
90
     B = params.B;
91
     C = params.C;
^{92}
     R = params.R;
93
     MW = params.MW;
^{94}
     G = params.G;
95
     C1 = params.C1;
96
     C2 = params.C2;
97
    C3 = params.C3;
98
```

```
C4 = params.C4;
99
     C5 = params.C5;
100
     C6 = params.C6;
101
102
     %% Algebraic equations
103
104
     P1 = \exp(A - B/(T1 - C));
105
     Z1 = 0.955 + 0.0*T1;
106
107
     HS1 = HH1/(N^2.19);
108
     FG1S= (N^1.56)*(C11*HS1 - C12)/(HS1 - C13);
109
     FG1 = FG1S*MW*P1*100/(T1*R*Z1);
110
111
     % ------
112
113
     P2 = \exp(A - B/(T2 - C));
114
     FG2 = XV1*CV1*sqrt(P2-PA);
115
116
     TB = (TA*FG1 + T2*FG2)/(FG1+FG2);
117
118
     Z2 = 0.566 + 1.26E - 3 \times TB;
119
     % ------
120
121
     P3 = \exp(A - B/(TD - C));
122
     Z3 = -0.194 + 2.97E - 3*TD;
123
124
     HS2 = HH2/(N^2.11);
125
     TX = C21/(tan((C22-HS2)/C23));
126
     FG3S = (N^{1.79})*(C24 + C25*log(sqrt(TX^{2}+1)-TX));
127
     FG3 = FG3S*MW*PA*100/(TB*R*Z2);
128
129
     % -----
130
     % Enthalpies
131
     HFG1 = 747.441 + 1.36908*T1;
132
     HFG2 = 663.375 + 1.63599 * T2;
133
     HFG3 = 474.018 + 2.09759 * TC;
134
135
     HFL2 = 7.16036 + 2.63768*T2;
136
     HFL3 = 95.5601 + 2.32367 * T3;
137
     HFL4 = 95.5601 + 2.32367 * TD;
138
139
     HW1V = 747.441 + 1.36908*T1;
140
     HW1L = 7.16036 + 2.63768*T1;
141
142
     HW2V = 663.375 + 1.63599 * T2;
143
     HW2L = 7.16036 + 2.63768 * T2;
144
145
     % ------
146
147
     A1 = \exp(-U1A1/FCP1);
148
     TP10 = (1-A1)*T1 + A1*TP1I;
149
     Q1 = FCP1*(TP1I - TP10)
150
151
     A2 = \exp(-U2A2/FCP2);
152
```

```
TP20 = (1-A2)*T2 + A2*TP2I;
153
      Q2 = FCP2*(TP2I - TP20)
154
155
      A3 = \exp(-U3A3/FCP3);
156
      TP30 = (1-A3)*TD + A3*TP3I;
157
      QC = FCP3*(TP3I - TP30);
158
159
     % -----
160
161
      FL2 = XV2*CV2*sqrt(P2-P1);
162
     FL3 = XV3*CV3*sqrt(P3-P2);
163
      FL4 = -QC/(HFG3-HFL4);
164
165
      ETA1 = E11*HS1 + E12 - 10^{(E13*HS1 - E14)};
166
167
      CPI1 = C1 + C2*T1*(C3 + C4*T1*(C5 + C6*T1));
168
      CP01 = C1 + C2*TA*(C3 + C4*TA*(C5 + C6*TA));
169
170
      G1 = 0.5*(CPI1/(CPI1-R) + CPO1/(CPO1-R));
171
172
      POL1 = ETA1*G1/(G1-1);
173
     ETA2 = E21*HS2 + E22 - 10^{(E23*HS2 - E24)};
174
175
      CPI2 = C1 + C2*TB*(C3 + C4*TB*(C5 + C6*TB));
176
      CPO2 = C1 + C2*TC*(C3 + C4*TC*(C5 + C6*TC));
177
178
      G2 = 0.5*(CPI2/(CPI2-R) + CPO2/(CPO2-R));
179
      POL2 = ETA2*G2/(G2-1);
180
181
      WL1 = W1 - WV1;
182
      WL2 = W2 - WV2;
183
      W3 = W - W1 - W2 - W4;
184
185
     HL1 = WL1*HW1L;
186
      HV1 = WV1 * HW1V;
187
188
      HL2 = WL2 * HW2L;
189
      HV2 = WV2 * HW2V;
190
191
      VF1 = 8.05418E-4 + 3.934E-6*T1;
192
      VF2 = 5.91479E-4 + 4.777E-6*T2;
193
      VF3 = -2.00589E - 4 + 7.493E - 6*TD;
194
195
      V1G = V1 - WL1 * VF1;
196
      V2G = V2 - WL2*VF2;
197
      V4G = V3 + VC - W3*VF3;
198
199
      VG1 = V1G/WV1;
200
      VG2 = V2G/WV2;
201
      VG4 = V4G/W4;
202
203
204
     L1 = WL1 * VF1;
     L2 = WL2 * VF2;
205
     L3 = W3 * VF3;
206
```

```
207
     PTH1 = 0.5*FG1*(CP01+CPI1)*(TA-T1)*1000/MW;
208
     PTH2 = 0.5*FG3*(CP02+CP12)*(TC-TB)*1000/MW;
209
     PTHTOT = PTH1 + PTH2;
210
211
     %% Defining the derivatives
212
213
     dH1 = HFL2*FL2 - HFG1*FG1 + Q1;
214
     dH2 = HFL3*FL3 - HFL2*FL2 - HFG2*FG2 + Q2;
215
     dT3 = FL4*(TD - T3)/W3;
216
     dW1 = FL2 - FG1;
217
     dW2 = FL3 - FL2 - FG2;
218
     dW4 = FG3 - FL4;
219
220
     dx = [dH1; dH2; dT3; dW1; dW2; dW4];
221
222
     %% Defining the residuals
223
224
     % Algebraic
225
226
     T1resid = H1 - HL1 - HV1;
     T2resid = H2 - HL2 - HV2;
227
     PAresid = FG3 - FG1 - FG2;
228
     TAresid = TA - T1*((PA/P1)^{(1/POL1)});
229
     TCresid = TC - TB*((P3/PA)^(1/POL2));
230
231
     TDresid = P3 - Z3*R*TD/(MW*VG4*100);
     HH1resid = HH1 - POL1*(R*1000/(G*MW))*(TA - T1);
232
     HH2resid = HH2 - POL2*(R*1000/(G*MW))*(TC - TB);
233
     WV1resid = P1 - Z1*R*T1/(MW*VG1*100);
234
     WV2resid = P2 - Z2*R*T2/(MW*VG2*100);
235
236
     % Controllers
237
     KcL1C = 0.5;
238
     L1Cresid = (0.2441 - XV2) + (L1sp - L1)*KcL1C;
239
240
     KcL2C = 0.6;
241
     L2Cresid = (0.2961 - XV3) + (L2sp - L2)*KcL2C;
242
243
     resids = [T1resid; T2resid; PAresid; TAresid; TCresid; TDresid;...
244
               HH1resid; HH2resid; WV1resid; WV2resid; L1Cresid; L2Cresid;...
245
               ];
^{246}
247
     % Dummies
248
     L1resid = L1-L1dummy;
249
     L2resid = L2-L2dummy;
250
     L3resid = L3-L3dummy;
251
252
     P1resid = P1-P1dummy;
253
254
     P2resid = P2-P2dummy;
     P3resid = P3-P3dummy;
255
256
     TP10resid = TP10-TP10dummy;
257
258
     TP2Oresid = TP2O-TP2Odummy;
     TP3Oresid = TP3O-TP3Odummy;
259
260
```

```
FG1resid = FG1-FG1dummy;
261
     FG2resid = FG2-FG2dummy;
262
     FG3resid = FG3-FG3dummy;
263
264
     FL2resid = FL2-FL2dummy;
265
     FL3resid = FL3-FL3dummy;
266
     FL4resid = FL4-FL4dummy;
267
268
     TBresid = TB-TBdummy;
269
270
     resids = [resids; L1resid; L2resid; L3resid; P1resid; P2resid; P3resid; ...
271
                TP1Oresid; TP2Oresid; TP3Oresid; FG1resid; FG2resid; FG3resid;...
272
                FL2resid; FL3resid; FL4resid; TBresid];
273
274
     %% Output
275
276
     out = [dx; resids];
277
278
     end
279
```

#### Initialisation of the parameters

Creates struct of parameters.

```
function params = init_params()
1
2
     % Refrigerant inventory [kg]
3
     params.W = 6500;
4
\mathbf{5}
     % Vessels sizes [m3]
6
     params.V1 = 20; % LP evaporator
7
     params.V2 = 3.393; % IP evaporator
8
     params.V3 = 18.85; % Receiver
9
     params.VC = 4.15; % Condenser
10
11
     % Coefficients for curve fittings for first compressor performance
12
     params.C11 = 1.9928;
13
     params.C12 = 16791;
14
     params.C13 = 8756.4;
15
16
     % Coefficients for curve fittings for second compressor performance
17
     params.C21 = 0.45615;
18
     params.C22 = 10296;
19
     params.C23 = 2956.2;
20
     params.C24 = 0.816051;
^{21}
     params.C25 = 0.27585;
22
23
     % Coefficients for curve fittings for first compressor isentropic efficiency
^{24}
     params.E11 = 6.47E-5;
^{25}
     params.E12 = 0.353;
26
     params.E13 = 7.101E-4;
27
     params.E14 = 6.5963;
28
29
     % Coefficients for curve fittings for second compressor isentropic efficiency
30
     params.E21 = 4.098E-5;
31
```

```
params.E22 = 0.364;
32
    params.E23 = 1.121E-3;
33
    params.E24 = 12.445;
34
35
     \% Combined overall heat transfer coefficients and heat transfer areas
36
    % in the two evaporators and the condenser [J/(s.K)]
37
    params.U1A1 = 146.066; % LP evaporator
38
    params.U2A2 = 5.5479; % IP evaporator
39
    params.U3A3 = 420.643; % Condenser
40
41
    % Valve constants [kg/(s.bar0.5)]
42
    params.CV1 = 3.39814; % Vapour valve
43
    params.CV2 = 2.233338; % First liquid valve
44
    params.CV3 = 1.85435; % Second liquid valve
^{45}
46
    % Combined process stream flowrate and specific heat capacity [J/(s.K)]
47
    params.FCP1 = 111.394; % LP evaporator
^{48}
    params.FCP2 = 24.32; % IP evaporator
^{49}
50
    % Process stream inlet temperatures [K]
51
    params.TP1I = 235.2; % Process stream in LP evaporator
52
    params.TP2I = 280.4; % Process stream in IP evaporator
53
    params.TP3I = 303.0; % Cooling air in the condenser
54
55
56
    % Antoine Equation coefficients for propylene
    params.A = 9.0825;
57
    params.B = 1807.53;
58
    params.C = 26.15;
59
60
    % General constants
61
    params.R = 8.314; % Gas constant [J/(mol.K)]
62
    params.MW = 42.081; % Propylene molecular weight [kg/kmol]
63
    params.G = 9.81; % Gravity acceleration [m/s2]
64
65
     % Specific heat capacity equation coefficients for propylene
66
    params.C1 = 3.707;
67
    params.C2 = 0.01;
68
    params.C3 = 23.439;
69
    params.C4 = 0.001;
70
    params.C5 = -11.594;
^{71}
    params.C6 = 2.2033E-3;
72
73
    end
74
```

#### B.2 Integrator

Integrates the model using ode15s. First call to follow is to create good initial values for the integrator, but this step seems unnecessary.

```
7
     % Initial estimates for the states
8
9
     % Differential states
10
     W1ic = 1.8790e+03;
11
     W2ic = 509.5381;
12
     T3ic = 310.3064;
13
     H1ic = 1.1346e+06;
14
     H2ic = 3.6506e+05;
15
     W4ic = 524.1002;
16
17
     x0_diff = [H1ic; H2ic; T3ic; W1ic; W2ic; W4ic]; % Diff.
^{18}
19
     % Algebraic states
20
     T1ic = 222.8800;
^{21}
     T2ic = 262.5103;
^{22}
     PAic = 3.8933;
^{23}
     TAic = 295.0822;
^{24}
     TCic = 358.1332;
^{25}
     TDic = 310.3064;
26
     HH1ic = 7.5895e+03;
^{27}
     HH2ic = 8.7647e+03;
^{28}
     WV1ic = 36.1681;
^{29}
     WV2ic = 21.8629;
30
^{31}
     XV2ic = 0.7000;
32
     XV3ic = 0.7096;
33
34
     x0_alg = [T1ic; T2ic; PAic; TAic; TCic; ...
35
         TDic; HH1ic; HH2ic; WV1ic; WV2ic; XV2ic; XV3ic]; % Alg.
36
37
     % Additional (non-state) variables
38
     L1ic
               = 3.1;
39
     L2ic
               = 0.9;
40
     L3ic
               = 7.6216;
^{41}
42
     P1ic
               = 0.9;
43
     P2ic
               = 4.2;
^{44}
     P3ic
               = 15.2025;
45
46
     TP10ic
              = 226.2000;
47
     TP20ic
              = 276.7510;
^{48}
     TP30ic
              = 308.1249;
49
50
     FG1ic
               = 2.8400;
51
     FG2ic
               = 1.5245;
52
     FG3ic
              = 4.3646;
53
54
              = 2.8400;
     FL2ic
55
     FL3ic
               = 4.3646;
56
     FL4ic
               = 4.3646;
57
58
     TBic
               = 283.7050;
59
60
```

```
x0_add = [L1ic; L2ic; L3ic; P1ic; P2ic; P3ic; TP10ic; TP20ic; TP30ic; ...
61
         FG1ic; FG2ic; FG3ic; FL2ic; FL3ic; FL4ic; TBic];
62
63
     x0 = [x0_diff; x0_alg; x0_add]; % Combining diff, alg and additional
64
65
     % Initial conditions for the inputs
66
     L1spic = 4.0118;
67
     L2spic = 1.5892;
68
     Nic
            = 0.9912:
69
     XV1ic = 0.8097;
70
     FCP3ic = 348.00;
71
72
     u0 = [L1spic; L2spic; Nic; XV1ic; FCP3ic];
73
^{74}
     % Calculating the steady state
75
     g = @(x) model([],x,u0);
76
77
     x_SS = fsolve(g, x0);
78
79
     80
     %% Calculating responses to disturbances / setpoint changes
81
     82
83
     % Doing a step change in L1 setpoint
84
     u = u0:
85
     %u(1) = u(1)*1.1;
86
87
     % Parametrizing the function to pass extra parameters to it (u and params)
88
     params = init_params;
89
     %params.TP1I = params.TP1I*1.05;
90
     g = @(t,x) model(t,x,u,params);
91
92
     % Defining the constant, singular mass matrix M
93
     M = diag([ones(1,length(x0_diff)),zeros(1,length(x0_alg)+length(x0_add))]);
^{94}
95
     J = Q(t,x) jac(t,x,u);
96
97
     % Setting the options for the ODEsolver
98
     %options = odeset('Jacobian', J, 'Mass', M, 'MStateDependence', 'none',...
99
          'MassSingular', 'yes', 'RelTol', 1e-4, 'Vectorized', 'off');
     %
100
101
      options = odeset('Mass',M,'MStateDependence', 'none',...
102
          'MassSingular', 'yes', 'RelTol', 1e-4, 'Vectorized', 'off');
103
104
     tspan = [0:0.5:2000];
105
     [t,x] = ode15s(g,tspan,x_SS,options);
106
107
     % Calculating the corresponding outputs from the states
108
     L1 = x(:, 19);
109
     L2 = x(:, 20);
110
     L3 = x(:,21);
111
112
     P1 = x(:,22);
     P2 = x(:,23);
113
    P3 = x(:,24);
114
```

```
T1 = x(:,7);
115
      T2 = x(:,8);
116
117
      T3 = x(:,3);
      TP10 = x(:, 25);
118
      TP20 = x(:, 26);
119
      TP30 = x(:, 27);
120
      FG2 = x(:, 29);
121
      FL2 = x(:, 31);
122
      FL3 = x(:, 32);
123
124
      % Plotting the results
125
      figure()
126
127
      hold on
128
      subplot(5,3,1); plot(t,L1)
129
      xlabel('t'); ylabel('L1')
130
      subplot(5,3,2); plot(t,L2)
131
      xlabel('t'); vlabel('L2')
132
      subplot(5,3,3); plot(t,L3)
133
134
      xlabel('t'); ylabel('L3')
      subplot(5,3,4); plot(t,P1)
135
      xlabel('t'); ylabel('P1')
136
      subplot(5,3,5); plot(t,P2)
137
      xlabel('t'); ylabel('P2')
138
139
      subplot(5,3,6); plot(t,P3)
      xlabel('t'); ylabel('P3')
140
      subplot(5,3,7); plot(t,T1)
141
      xlabel('t'); ylabel('T1')
142
      subplot(5,3,8); plot(t,T2)
143
      xlabel('t'); ylabel('T2')
144
145
      subplot(5,3,9); plot(t,T3)
      xlabel('t'); ylabel('T3')
146
      subplot(5,3,10); plot(t,FG2)
147
      xlabel('t'); ylabel('FG2')
148
      subplot(5,3,11); plot(t,FL2)
149
      xlabel('t'); ylabel('FL2')
150
      subplot(5,3,12); plot(t,FL3)
151
      xlabel('t'); ylabel('FL3')
152
      subplot(5,3,13); plot(t,TP10)
153
      xlabel('t'); ylabel('TP10')
154
      subplot(5,3,14); plot(t,TP20)
155
      xlabel('t'); ylabel('TP20')
156
      subplot(5,3,15); plot(t,TP30)
157
      xlabel('t'); ylabel('TP30')
158
     hold off
159
160
      end
161
```

#### B.3 Steady-state optimization

Optimizing the model using fmincon.

```
1 function [y,fval,exitflag] = opt(u0,x0,params)
2
3 if (~exist('params','var'))
```

```
params = init_params();
4
     \operatorname{end}
5
6
     if (~exist('u0','var')) || isempty(u0)
\overline{7}
         % Inputs
8
         L1spic = 4.0118;
9
         L2spic = 1.5892;
10
         Nic
                 = 0.9912;
11
         XV1ic = 0.8097;
12
         FCP3ic = 348.00;
^{13}
         u0 = [L1spic; L2spic; Nic; XV1ic; FCP3ic];
14
     end
15
     if (~exist('x0','var')) || isempty(x0)
16
17
         % Differential states
         H1ic = 1.1346e+06;
18
         H2ic = 3.6506e+05;
19
         W1ic = 1.8790e+03;
^{20}
         W2ic = 509.5381;
^{21}
         T3ic = 310.3064;
22
         W4ic = 524.1002;
23
         x0_diff = [H1ic; H2ic; T3ic; W1ic; W2ic; W4ic];
                                                                       % Differential
^{24}
25
         % Algebraic states
26
         T1ic = 222.8800;
27
28
         T2ic = 262.5103;
         PAic = 3.8933;
29
         TAic = 295.0822;
30
         TCic = 358.1332;
31
         TDic = 310.3064;
32
         HH1ic = 7.5895e+03;
33
         HH2ic = 8.7647e+03;
34
         WV1ic = 36.1681;
35
         WV2ic = 21.8629;
36
         XV2ic = 0.7000;
37
         XV3ic = 0.7096;
38
         x0_alg = [T1ic; T2ic; PAic; TAic; TCic; ...
39
                      TDic; HH1ic; HH2ic; WV1ic; WV2ic; XV2ic; XV3ic]; % Algebraic
40
41
         % Additional (non-state) variables
42
                   = 3.1;
         L1ic
^{43}
         L2ic
                   = 0.9;
44
         L3ic
                   = 7.6216;
45
         P1ic
                   = 0.9;
46
         P2ic
                   = 4.2;
47
                   = 15.2025;
         P3ic
^{48}
                   = 226.2000;
         TP10ic
49
         TP20ic
                   = 276.7510;
50
         TP30ic
                   = 308.1249;
51
         FG1ic
                   = 2.8400;
52
         FG2ic
                   = 1.5245;
53
         FG3ic
                   = 4.3646;
54
         FL2ic
                   = 2.8400;
55
         FL3ic
                   = 4.3646;
56
         FL4ic
                   = 4.3646;
57
```

```
TBic
                    = 283.7050;
58
          x0_add = [L1ic; L2ic; L3ic; P1ic; P2ic; P3ic; TP10ic; TP20ic; ...
59
            TP30ic; FG1ic; FG2ic; FG3ic; FL2ic; FL3ic; FL4ic; TBic]; % Additional
60
61
          x0 = [x0_diff; x0_alg; x0_add];
                                               % Combining diff, alg and additional
62
     end
63
64
     g = @(x) model([],x,u0,params);
65
66
     x0 = fsolve(g,x0); % Get initial guess
67
68
     y0 = [u0; x0]; % Combining inputs and states
69
70
71
     %% Constraints
     lb=zeros(length(y0),1);
72
     1b(3) = 0.0; \% N
73
     1b(4) = 0; \% XV1
^{74}
     1b(5) = 116; \% FCP3
75
     1b(22) = 0; \% XV2
76
     1b(23) = 0; \% XV3
77
     lb(24) = 2.9; % L1
78
     1b(25) = 0.6; \% L2
79
     1b(26) = 6.9; \% L3
80
     lb(27) = 0; % P1
81
82
     1b(28) = 3; \% P2
     1b(29) = 12; % P3
83
     lb(30) = 200; % TP10
84
     1b(34) = 0; \% FG2
85
     1b(36) = 0; \% FL2
86
     1b(37) = 0; \% FL3
87
88
     ub=ones(length(y0),1)*1e12;
89
     ub(3) = 1.1; \% N
90
     ub(4) = 1; \% XV1
91
     ub(5) = 348; \% FCP3
^{92}
     ub(22) = 1; \% XV2
93
     ub(23) = 1; \% XV3
94
     ub(24) = 6.4; \% L1
95
     ub(25) = 1.6; \% L2
96
     ub(26) = 13.7; % L3
97
     ub(27) = 2; \% P1
98
     ub(28) = 6; % P2
99
     ub(29) = 18; % P3
100
     ub(30) = 300; % TP10
101
     ub(34) = 6.31; \% FG2
102
     ub(36) = 5.47; \% FL2
103
     ub(37) = 7.18; \% FL3
104
105
     %% Optimization
106
107
     % fmincon options
108
109
     alg = 'Interior-Point';
     %alg = 'sqp';
110
     options = optimset('TolFun',10e-7,'TolCon',10e-7,'MaxFunEvals',1e4,...
111
```

```
'MaxIter', 1e4, 'Display', 'none', 'Algorithm', alg, 'Diagnostics', 'off'...
112
      );
113
114
      % Call fmincon to optimize the model
115
      nlconpar = @(y) nlcon(y,params);
116
      [y,fval,exitflag] = fmincon(@cost,y0,[],[],[],lb,ub,nlconpar,options);
117
118
      name = {'L1sp', 'L2sp', 'N', 'XV1', 'FCP3', 'H1', 'H2', 'T3', 'W1', 'W2', 'W4',...
119
               'T1', 'T2', 'PA', 'TA', 'TC', 'TD', 'HH1', 'HH2', 'WV1', 'WV2', 'XV2',...
120
               'XV3','L1','L2','L3','P1','P2','P3','TP10','TP20','TP30','FG1',...
121
               'FG2', 'FG3', 'FL2', 'FL3', 'FL4', 'TB'...
122
              };
123
124
      if exitflag ~= 1
125
          fprintf('Exitflag not equal to 1! \n\n')
126
      end
127
128
      upper_limit = abs(ub./y)-1;
129
      lower_limit = 1-abs(lb./y);
130
      err_tol = 1e-7;
131
      for i = 1:length(y0)
132
          if upper_limit(i) < err_tol</pre>
133
               fprintf('Active constraint: %s at upper limit \n',name{i})
134
          elseif lower_limit(i) < err_tol</pre>
135
               fprintf('Active constraint: %s at lower limit \n',name{i})
136
          end
137
      end
138
139
      function [j] = cost(y)
140
141
142
      %% Objective function
143
      % Unpacking the parameters
144
      T1 = y(12);
145
      TA = v(15);
146
      TB = y(39);
147
      TC = y(16);
148
      FG1 = y(33);
149
      FG3 = y(35);
150
151
      %% Calculating the cost
152
153
      % General constants
154
      MW = 42.081;
155
156
      \% Specific heat capacity equation coefficients for propylene
157
      C1 = 3.707;
158
      C2 = 0.01;
159
      C3 = 23.439;
160
      C4 = 0.001;
161
      C5 = -11.594;
162
      C6 = 2.2033E-3;
163
164
     CPI1 = C1 + C2*T1*(C3 + C4*T1*(C5 + C6*T1));
165
```

```
CP01 = C1 + C2*TA*(C3 + C4*TA*(C5 + C6*TA));
166
167
      CPI2 = C1 + C2*TB*(C3 + C4*TB*(C5 + C6*TB));
168
      CPO2 = C1 + C2*TC*(C3 + C4*TC*(C5 + C6*TC));
169
170
      % Energy consumption
171
      PTH1 = 0.5*FG1*(CP01+CPI1)*(TA-T1)*1000/MW:
172
      PTH2 = 0.5*FG3*(CP02+CPI2)*(TC-TB)*1000/MW;
173
      PTHTOT = PTH1 + PTH2;
174
175
      j = PTHTOT;
176
177
      function [c ,ceq ] = nlcon(y,params)
178
179
      % Inputs
180
      u = y(1:5);
181
      % State variables
182
      x = y(6:end);
183
184
      % Nonlinear inequality constraints C(x)<0
185
      c=[x(25)-226.2,...
186
         x(26) - 276.751];
187
188
      % Nonlinear equality constraints C(x)=0
189
      ceq=[model([],x,u,params);...
190
          y(24)-3.1 ; ...
191
          y(25)-0.9 ; ...
192
          ];
193
194
```

#### B.4 Finding active constraint regions

```
A1int = linspace(5, 55, 101);
1
     A2int = linspace(5, 55, 101);
2
3
     map1 = zeros(length(A1int),length(A2int));
4
     map2 = zeros(length(A1int),length(A2int));
5
     map3 = zeros(length(A1int),length(A2int));
6
7
     for i = 1:length(A1int)
8
         for j = 1:length(A2int)
9
              try
10
                  p = init_params;
11
                  p.U1A1 = A1int(i);
12
                  p.U2A2 = A2int(j);
13
                  [y,fval,exit,cvu,cvd] = opt(u0,x0,p);
14
                  if exit > 0
15
                      map1(i,j) = cvu;
16
                      map2(i,j) = cvd;
17
                      map3(i,j) = fval;
18
                  else
19
                      map1(i,j) = exit;
20
                      map2(i,j) = exit;
^{21}
                  end
^{22}
```

```
catch err
23
                    if strcmp(err.identifier,'optim:barrier:UsrNonlConstrUndefAtX0')
^{24}
                         map1(i,j) = -10;
25
                         map2(i,j) = -10;
26
                    else
27
                         rethrow(err)
28
                    end
29
               \operatorname{end}
30
          end
31
     end
^{32}
     combimap = (map1+map2*1i);
33
     for i = 1:101
^{34}
          for j = 1:101
35
               Z(i,j) = getflag(combimap(i,j));
36
          end
\mathbf{37}
     end
38
     X = A1int;
39
     Y = A2int;
40
     h = pcolor(Y,X,Z);
^{41}
     set(h, 'EdgeColor', 'none');
42
     function flag = getflag(z)
1
2
               switch z
                    case -10 - 10i;
3
                             flag = -1;
4
                    case 0;
\mathbf{5}
                         flag = -1;
6
                    case -2 - 2i
\overline{7}
                         flag = -1;
8
                    case 0 + 32i
9
                         flag = 1;
10
                    case 56
11
                         flag = 2;
12
                    case 4194304
13
                         flag = 3;
14
                    case 4194312
15
                         flag = 4;
16
                    case 4194320
17
                         flag = 5;
^{18}
                    case 4194344
19
                         flag = 6;
20
                    case 4194352
^{21}
                         flag = 7;
^{22}
                    case 8388632
23
                         flag = 8;
^{24}
                    case 8388664
25
                         flag = 9;
26
                    case 12582920
27
                         flag = 10;
28
                    case 12582928
29
                         flag = 11;
30
                    case 12582952
31
                         flag = 12;
^{32}
                    case 12582960
33
```

```
flag = 13;
^{34}
                     case 4194304 + 16777216i
35
                         flag = 14;
36
                     case 0 + 67108864i
\mathbf{37}
                         flag = 15;
38
                    case 16 + 67108864i
39
                         flag = 16;
40
                     case 536870912
41
                         flag = 17;
^{42}
                     case 536870912 + 67108864i
^{43}
                         flag = 18;
^{44}
                     case 545259536
45
                         flag = 19;
46
                     case 545259544
47
                         flag = 20;
^{48}
                     case 549453840
49
                         flag = 21;
50
                    otherwise
51
                         fprintf('unknown z: %14.14f, %14.14f\n',real(z),imag(z))
52
                         flag = 0;
53
               end
54
          end
55
56
57
58
59
60
61
62
63
64
65
66
\mathbf{67}
68
69
70
71
72
73
74
75
76
77
^{78}
79
```