Rheinisch–Westfälische
Technische Hochschule
Aachen

Lehrstuhl für Prozesstechnik
Professor Dr.–Ing. Wolfgang Marquardt

Expansion and examination of the stationary model of an ammonia refrigeration cycle with emphasis on optimal operation / self-optimizing control

External Project Work

by
Johannes Jäschke

Supervisors:
Professor S. Skogestad
Dipl.–Ing. Arndt Hartwich
Siv.–Ing Jørgen B. Jensen

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Abstract

In industrial processes, especially in cyrogenic processes, vapour compression cycles have become more and more complex due to high demands on the thermodynamic efficiency. Operation and control of these systems are strongly influenced by this complexity. Hence, to ensure optimal operation of these complex systems, it is necessary to fully understand the principles in simple cases.

The subject of this project is to extend a stationary model of a simple ammonia refrigeration cycle by including internal heat exchange and to study this model with respect to optimal operation and self-optimizing control. This implies finding a set of controlled variables, which when kept at constant setpoints, indirectly leads to near-optimal operation with acceptable loss.

In a first step the design specifications are developed and the difference between optimal design (finding equipment) and optimal operation (given equipment) is elaborated.

The model is studied and the operation is optimized under various conditions (disturbances). Then the operation of the cycle is checked with respect to self-optimizing control and evaluated.

The model is then augmented by introducing an internal heat exchanger and implemented in MATLAB. It is found, that internal heat exchange is not the thermodynamic optimum for this ammonia cooling processes.

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Symbol	Explanation	Unit
Δh_v	Latent heat for vaporization at reference conditions	[J/g]
$\Delta T_{con,end}$	Temperature difference between ambient and condenser outlet	[K]
ΔT_{min}	Minimum temperature difference in heat exchanger	[K]
ΔT_{sub}	Amount of subcooling	[K]
ΔT_{sup}	Amount of superheating	[K]
ω	Reduced temperature	[–]
ρ_l	Liquid density	[g/cm^3]
ρ_v	Vapor density	[g/cm^3]
$A_{con,tot}$	Total condenser Area	[m^2]
$A_{con,tot}$	Total condenser heat tranfer area	[m^2]
A_{design}	Heat transfer area obtained from optimal design	[m^2]
A_{ihx}	Total internal heat exchanger heat tranfer area	[m^2]
A_{vap}	Total evaporator heat tranfer area	[m^2]
$A_1 - A_5$	Coefficients for the fluid model	[–]
A_i	Heat exchange area i	[m^2]
A	Area	[m^2]
$c_{p,g}$	Vapour heat capacity	[J/gK]
$c_{p,l}$	Liquid heat capacity	[J/gK]
c_s	controlled variable at constant setpoint	[–]
C_v	Valve constant	[–]
c	Controlled variables	[various]
d^*	nominal disturbance (nominal condition)	[–]
d	Disturbance	[K]
G'	Scaled linear gain	[–]
G	Linear gain	[various]
h_g	Vapour enthalpy	[J/g]
h_i	enthalpy at point i	[J/g]
h_l	Liquid enthalpy	[J/g]
$J_{opt}(d)$	Reoptimizend cost at full disturbance	[W]
$J(u,d)$	Cost at full disturbance d	[W]
J	Cost function	[W]
L_u	Loss at full disturbance d	[W]

Continued

Symbol	Explanation	Unit
L	Loss	[W]
m	Manipulated variables	[–]
$\dot{n}$	Flowrate	[mol/sec]
N	Holdup	[mol]
$N_{con,l}$	Condenser liquid holdup	[mol]
$N_{con,v}$	Condenser vapor holdup	[mol]
n	Noise	[various]
Na	Liquid holdup in internal heat exchanger	[mol]
Nb	Vapor holdup in internal heat exchanger	[mol]
P_h	High pressure	[Pa]
P_l	Low pressure	[Pa]
Q_c	Heat transferred at the cold side	[W]
Q_h	Heat transferred at the hot side	[W]
Q_i	Heat transferred at area i	[W]
R	Ideal gas constant	[J/gK]
$T_{c,des}$	Design cold (room) temperature	[K]
$T_{c,op}$	Operation cold (room) temperature	[K]
$T_{con,out}$	Condenser outlet temperature	[K]
T_{crit}	Critical temperature	[K]
$T_{h,des}$	Design warm ambient temperature	[K]
$T_{h,op}$	Operation warm (ambient) temperature	[K]
T_{ref}	Reference temperature for fluid model	[K]
T_c	Cold room temperature	[K]
T_h	Warm outside temperature	[K]
T_i	Temperature at point i in the process	[K]
Ta	Temperature in stream a	[K]
Tb	Temperature in stream b	[K]
u	Manipulated variables	[various]
U	Heat transfer coefficient	[W/m^{2}K]
$V_{con,tot,}$	Total condenser volume	[m^3]
$V_{ihx,tot,}$	Total internal heat exchanger volume	[m^3]

Continued

Symbol	Explanation	Unit
V_{vap}	Total evaporator volume	[m^3]
V_l	Liqiuid volume	[m^3]
V_v	Vapor volume	[m^3]
V	Volume	[m^2]
W_s	Shaft work	[J]
y	Nominal output variable	[–]
z	Valve opening	[–]

1 Introduction

Vapour compression cycles pumping heat from a low temperature to a high temperature have become a matter of course in our society. Modern life cannot be imagined without refrigerator or air conditioning. These applications vary in size from 1 kW to over 100 MW. They range from small ice boxes or car air conditioners to units which provide heating or cooling for entire buildings. The larger systems are usually found in industry. Especially the cryogenic industry demands large amounts of energy because a large amount of heat has to be transfered over a large temperature range. Examples for the use of these processes are the liquification of natural gas (LNG process) and air separation.

To exploit the thermodynamic possibilities as far as possible, more and more complex system designs are required. The thermodynamic efficiencies are improved by introducing more several pressure levels, mixing working fluids and arranging the cycles as a cooling cascade. A mixed fluid cascade (MFC) built by the Statoil Linde Technology Alliance in Snøhvit, Norway is shown in figure 1.1.

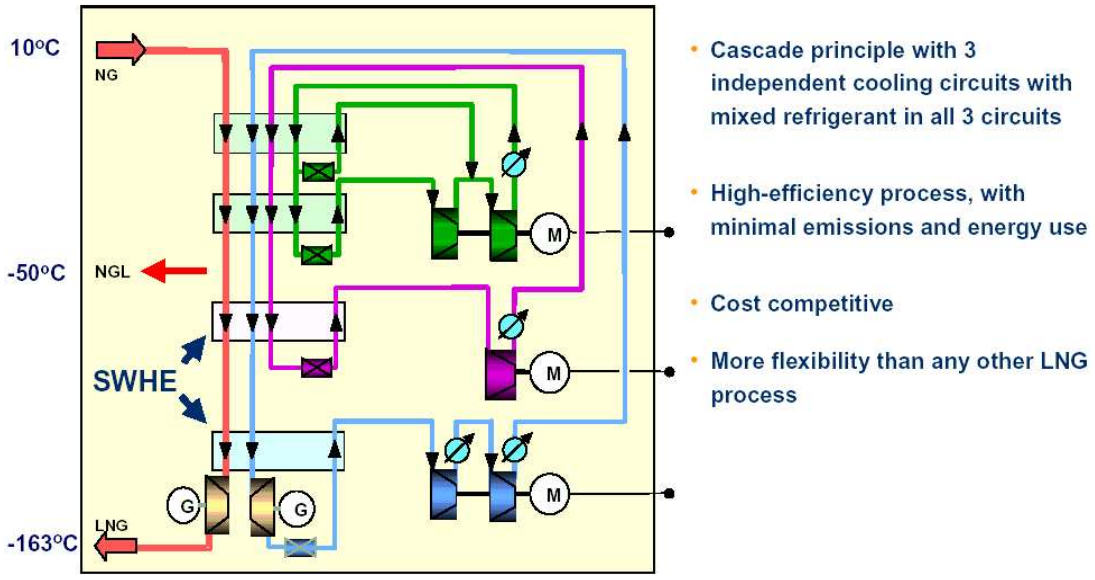

Figure 1.1: Schematic figure of the mixed fluid cascade built by the Statoil Linde Alliance in northern Norway (figure adapted from Dodson (2004))

Up to now many studies have been made considering optimal design of vapour com-

pression cycles, but far less work has been published dealing with optimal operation with given equipment.

There are different approaches to the problem of achieving optimal operation. Among them are the approach of dynamic optimization (**?**) and the approach of self-optimizing control (Skogestad (2000)). The latter approach implies finding a set of controlled variables which, when kept at constant setpoints, indirectly leads to near-optimal operation with acceptable loss. This strategy will be followed and applied in the course of this work.

The subject of this project is to examine an existing stationary model of a simple refrigeration unit and extend it by including internal heat exchange to find optimal design. Using this design the operation of the cycle is studied.

This work is believed to contribute to the objective of finding criteria for optimal operation of complex cryogenic vapour compression systems by giving an understanding of the basic cycles. However before this can be achieved it is necessary to understand the basic principles for simple cycles. These can later be applied to more complex structures.

2 Optimal operation

In this chapter, first some information on plant control structure is given. The basic principles are applicable to all kind of process control problems; however, where necessary they will be applied to the problem of the optimal control of a cooling process. In the second part the principle of self-optimizing control is explained and applied to a cooling process.

2.1 Control structure design

The control system of chemical plants can be subdivided into several layers, which are distinguished from each other by the time scale they operate in. A classification suggested by Skogestad (2000) is:

- Scheduling (weeks)
- Site-wide optimization (days)
- Local optimization (hours)
- Supervisory control (minutes)
- Regulatory control (seconds)

This structure is visualized in figure 2.1. The layers are connected by controlled variables c. The values of the variables c are calculated by the upper layer and implemented by the layer directly below.

Designing this control structure for a whole process plant is a very complex task. In order to design a control structure in the best possible way, a systematic approach has to be utilized. One of these systematic approaches is proposed by Skogestad (2004) and contains the following steps:

1. Selection of manipulated variables m;
2. Selection of controlled variables c;

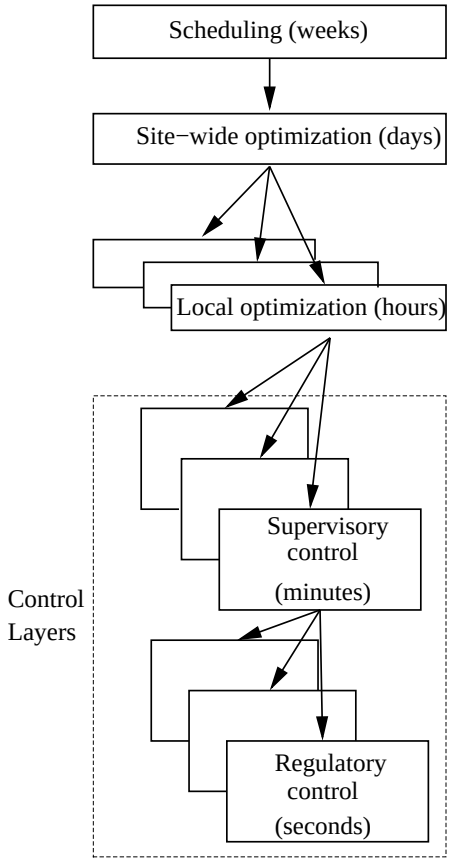

Figure 2.1: Control layers (adapted from Skogestad (2004))

3. Selection of measurements for control purposes including stabilization;

4. Selection of control configuration (structure of the overall controller that interconnects the controlled, manipulated and measured variables);

5. Selection of controller type (control law, specification, e.g. PID, decoupler, LQG)

Different model types are used for the analysis of the different layers. E.g. for the examination of the optimization layers generally a nonlinear steady state model is needed.[1]

When going one step further in control structure design, a dynamic model is needed to analyse the control layers. This analysis gives "secondary controlled variables", which

[1]There is an exception, in case of discontinuous (batch) processes a dynamic model is needed for the optimization layers.

ensure that the system does not drift away too far from the desired steady state operation point. Setting up a dynamic model for the refrigeration cycle considered here is the task following this work. In terms of points 1–5 of the systematic approach for control structure design, this thesis considers points 1 and 2, while the other points 3–5 are based on this work and have to be studied later.

2.2 Self-optimizing control

In order to quantitatively evaluate the control structure, a scalar cost function J is defined, which is to be minimized in operation. In real cases it is usually not possible to measure every disturbance online and to solve the optimization problem in real time. So it is of particular interest to find out, if it is possible to simplify the realization and still have acceptable performance. The loss L is defined as the difference between the actual cost and the optimal cost $L = J - J_{opt}$ with J_{opt} as the theoretical, reoptimized cost. From this aspect the term self-optimizing control is defined by Skogestad (2000) as follows:

> Self-optimizing control is when we can achieve an acceptable loss with constant setpoint values for the controlled variables (whithout the need to reoptimize when disturbances occur).

The cost related to different constant setpoints is shown in figure 2.2. It can easily be seen that the loss $L = J - J_{opt}$ is lower when c_{1s} is held constant than when c_{2s} is held constant. So c_{1s} is a good self optimizing variable.

However, there may be situations in which it is infeasible to hold a variable at a constant setpoint. This has to be taken into account when designing the control structure.

A strategy for finding the optimal control structure in the optimization layers is proposed by Skogestad (2000):

1. Degree of freedom analysis

   The degrees of freeodom for optimization are examined for the specific process.

2. Setting up the cost function and constraints

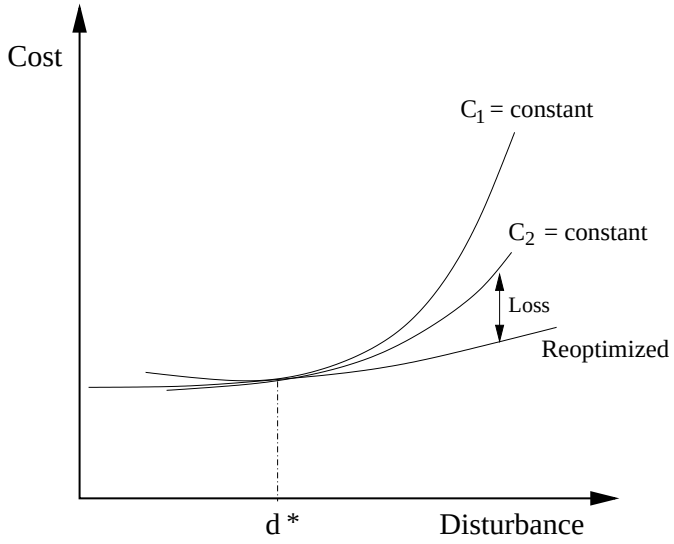

Figure 2.2: Cost function (adapted from Skogestad (2004))

This step contains the formulation of economic objectives and the constraints in terms of a scalar cost function J. This function should quantitatively represent how well the economic objectives are met. The factors contributing to this function can vary widely depending on the process and economic goals. A simple example for the cost function to minimize could be the energy or work applied to a process. More advanced cost functions may contain factors like e.g. the life time of a plant, safety issues, raw material consumption or CO_2 emission. Depending on the goal of the plant, there are numerous possibilities to formulate the cost function.

3. Identifying the important disturbances

   Here the system is examined, and disturbances which can arise are noted. Generally not only disturbances coming from outside the system are identified, but also errors in measurement, implementation and of other origin are taken into account.

4. Optimization

   The system is optimized for nominal conditions in step 4. After this step, all variable values of the system operating at nominal conditions are known.

5. Identifying candidate controlled variables

   To be identified as a candidate for a controlled variable at a constant setpoint in

step 5, the variables have to meet some requirements to ensure self-optimizing control (Skogestad and Postlethwaite (1996)): The optimal value should be insensitive to disturbances but sensitive to changes in the manipulated variables u. It should be easy to measure and control and, when more than one controlled variable is selected, they should not be closely correlated.

These requirements can be combined in the "Minimum singular value rule" (Skogestad (2000)): The model is linearized around the nominal operation point to

$$\Delta c = G\Delta u \tag{2.1}$$

for small disturbances. The variable u denotes the unconstrained degrees of freedom, c the candidates for controlled variables and G the linear gain. It is assumed that the controlled variable c has been scaled, so that the sum of its optimal range and the implementation error is unity. The variables u have been scaled in such a way, that a unit change has the same effect on the cost function J.

A set of good control candidates c is found by choosing it in such a way that the minimum singular value $\sigma(G)$ of the steady state gain matrix G is maximized. For a more detailed derivation see Skogestad (2000) and Skogestad and Postlethwaite (1996).

6. Evaluating loss at full disturbance

   As the model is linearized around the operating point to find the linear gain, this procedure can only indicate how good a candidate is for a disturbance close to nominal conditions. In a last step, the loss at full disturbance $L_u(u,d)$ with constant setpoints is checked to see how these candidats behave far from the nominal operating point:

$$L_u(u,d) = J_u(u,d) - J_{opt}(d) \tag{2.2}$$

   $J_u(u,d)$ is the cost at the disturbance d with constant setpoints and $J_{opt}(d)$ is the cost at the disturbance d when the system is fully reoptimized. If the loss $L_u(u,d)$ is acceptable, then self-optimizing control is achieved. In some cases, however, it may be found that a promising candidate is disqualified, because holding its setpoint constant at c_s far from nominal conditions is infeasible or leads to inacceptable loss.

3 The cooling process

Before presenting the mathematical relations for the model in the next chapter, the basic process is described briefly in this chapter. Figure 3.1 shows the principle of a simple cooling cycle. Vapor enters the compressor from the evaporator at a low pressure and is compressed to a high pressure level by applying the compressor work W_s. At high pressure and temperature the fluid is condensed and, if desired, subcooled by removing the heat Q_h at high temperature, before the pressure is reduced to its original level in an expansion choke with the valve opening z. The coolant is then vaporized at low pressure by applying the heat Q_c at low temperature and possibly overheated before entering the compressor again. More detailed information on the basics of refrigeration cycles can be found in Moran and Shapiro (1998) and Langley (2002).

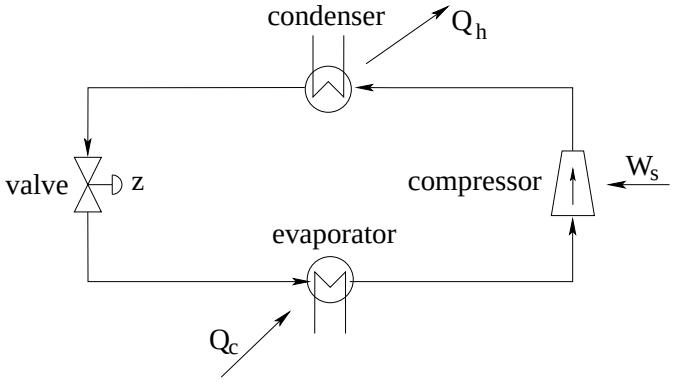

Figure 3.1: Simple cooling process

When implementing a process like this one, it is important to note that there are in fact differences between optimal design and optimal operation. Process equipment can not be designed optimal for all operating conditions. If the demands on a cooling device are to keep a room at a certain temperature, e.g. -10°C, the load will vary with the environment temperature.

For a simple, closed circuit as described above, there are five design specifications, i.e.: Load, high pressure level P_h, low pressure level P_l, amount of superheating ΔT_{sup} and amount of subcooling ΔT_{sub}. In operation mode, the specifications are different: The compressor work W_s, the valve opening z, and the product of the heat transfer coefficient UA in the two heat exchangers. Five parameters are specified in design, while

in operation only four are specified. The fifth unspecified degree of freedom corresponds to the pressure level, which is set indirectly by the charge, the amount of liquid in the heat exchangers. Depending on the design of the circuit, there is at most one degree of freedom to be used for optimization. The possibility of getting additional degrees of freedom by using bypasses for the heat exchangers exists, but this would be sub optimal and therefore this alternative is not considered further.

In operation there are two manipulated inputs, the compressor work W_s and the valve opening z. The compressor work W_s is used to set the load for the cycle, so it is not used for optimization. Depending on the design of the cycle the valve can be a degree of freedom for optimization. In a coventional evaporator the valve is used to control the amount of superheating in order to assure that only vapor is fed to the compressor.

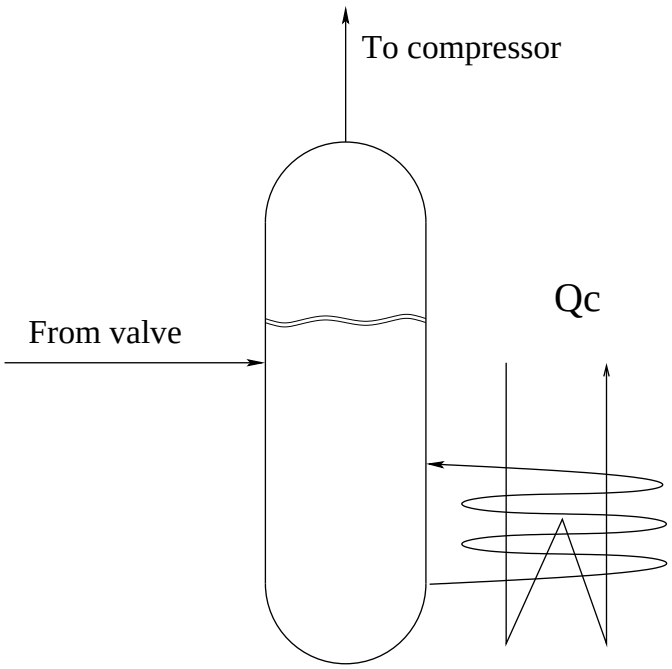

Figure 3.2: Principle of the flooded evaporator (adapted from Jensen and Skogestad (2005))

A design which has the advantage of fixing the amount of superheating without using the valve is the flooded evaporator design with floating liquid level, see figure 3.2. A flooded evaporator is characterized by the fact that all heat is applied to the liquid phase. This is advantageous, as the heat transfer coefficient to liquid is higher than to vapour.

The evaporator is designed in such a way that the floating liquid level is above the heat transfer area when the rest of the cooling system is flooded with the cooling fluid. But when the rest of the system is empty the liquid level is still below the vapor outlet. Thus it is ensured that no liquid enters the compressor. An evaporator built like this always produces saturated vapor,[1] regardless of the holdups in the rest of the system. This fact makes the valve available as a degree of freedom for optimization.

[1]Having saturated vapour entering the compresser might be undesired from a mechanical engineering point of view because of droplets damaging the compressor. But from a thermodynamic point of view superheating is not desirable as it reduces the coefficient of performance.

4 The mathematic models

4.1 The fluid model

The thermodynamic fluid model is taken from Haar and Gallagher (1978), and the relevant data is listed in Appendix B.2. The specific enthalpy h_l of the liquid is described by:

$$h_l(T) = c_{p,l}(T - T_{ref}) \tag{4.1}$$

It is a function of the difference between the temperature T and a reference temperature T_{ref}. The value for the reference temperature is $T_{ref} = 267.79\,\mathrm{K}$.

An additional term $\Delta_v h$ is added for the vapor enthalpy due to phase transition:

$$h_g(T) = c_{p,g}(T - T_{ref}) + \Delta_v h(T_{ref}) \tag{4.2}$$

The parameters $c_{p,l}$ and $c_{p,g}$ are the specific heat capacities for the liquid and vapour state, respectively.

The pressure P and temperature T in the heat exchangers are related by the saturation conditions. The saturation pressure as a function of temperature is calculated by the following expression:

$$\log_e\left(\frac{P}{P_c}\right) = \frac{1}{\omega}\left(A_1(1-\omega) + A_2(1-\omega)^{\frac{3}{2}} + A_3(1-\omega)^{\frac{5}{2}} + A_4(1-\omega)^5\right) \tag{4.3}$$

The variables in this equation are the reduced temperature $\omega = \frac{T}{T_{crit}}$ with T_{crit} as the critical temperature and P_c, the critical pressure. The coefficients A_1 to A_4 are taken from Haar and Gallagher (1978) and are listed in table B.2.

Finally, the vapour density is calculated using the ideal gas law with R being the ideal gas constant:

$$\rho_v = \frac{N}{V} = \frac{P}{\mathrm{R}T} \tag{4.4}$$

4.2 Simple model

In figure 4.1 a general illustration of a simple ammonia cooling circuit with a possible related pressure-enthalpy diagram is shown. The numbers 1 to 12 in the pressure-enthalpy diagram correspond to different regions in the cycle. As can be seen from the

figure, there is superheating (points 9 – 12) and subcooling (points 3 – 6). Depending on the practical design, not all attributes are present, but they are indicated here to introduce the notation in the model equations. Refrigerant entering the evaporator subcooled as indicated (point 7) is usually not desirable in practice. So a mixture of vapor and liquid is fed to the evaporator.

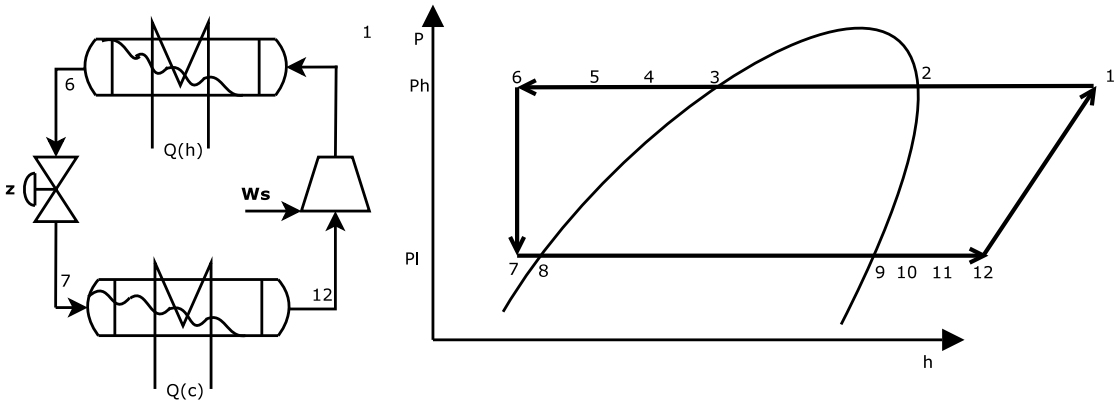

Figure 4.1: Schematic figure of the simple cycle with P-h-diagram

Using the flooded evaporator design, it is obvious that there can be no superheating at the outlet, i.e. points 9 – 12 in the pressure-enthalpy diagram coincide with point 9. From now on, all considerations in this project will be made to a system with a flooded evaporator.

4.2.1 Model equations

The model equations are kept simple to gain understanding of the process. They may be refined to more accurate relations later. All symbols used to describe this model can be found in the list of variables, page v.

The compressor

Compression is assumed adiabatic with the pressure-temperature relation:

$$\frac{T_{12}}{T_1} = \left[\frac{P_h}{P_l}\right]^{\frac{R}{c_{p,g}}} \tag{4.5}$$

Here T_1 and T_{12} is the temperature in Kelvin at point 1 and 12, and P_h and P_l are the pressures at high and low level, respectively.

The shaft work W_s is transferred to the liquid as described in equation 4.6:

$$W_s = \dot{n}(h_1 - h_{12}) \tag{4.6}$$

$\dot{n}$ is the molar flow rate, h_1 and h_{12} is the specific enthalpy of the fluid at point 1 and point 12, respectively.

The condenser

The condenser is designed as a cross flow heat exchanger which is devided into three sections, see figure 4.2. In the first section the vapour is cooled down to the saturation temperature. The arithmetic mean temperature is used to compute the transferred heat. The second condenser area contains the condensing vapour at saturation temperature. The third section of the condenser is the subcooling area, which is again divided into three control volumes for calculating the heat transfer.

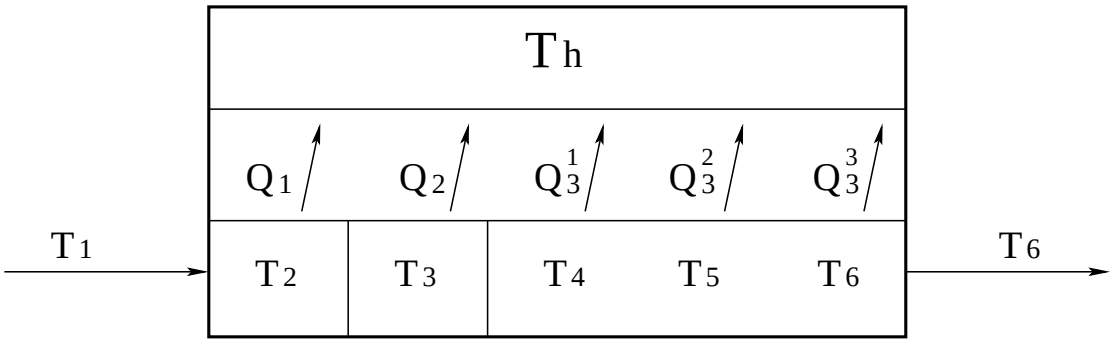

Figure 4.2: Schematic figure of the condenser with heat flows

The mathematic relations for the condenser are listed in equations 4.7 – 4.11.

$$Q_1 = UA_1 \left(T_h - \frac{T_1 + T_2}{2} \right) = \dot{n} \left(h_2 - h_1 \right) \tag{4.7}$$

$$Q_2 = UA_2 \left(T_h - T_3 \right) = \dot{n} \left(h_3 - h_2 \right) \tag{4.8}$$

$$Q_3^1 = \frac{UA_3}{3} \left(T_h - T_4 \right) = \dot{n} \left(h_4 - h_3 \right) \tag{4.9}$$

$$Q_3^2 = \frac{UA_3}{3} \left(T_h - T_5 \right) = \dot{n} \left(h_5 - h_4 \right) \tag{4.10}$$

$$Q_3^3 = \frac{UA_3}{3} \left(T_h - T_6 \right) = \dot{n} \left(h_6 - h_5 \right) \tag{4.11}$$

Q_i denotes the heat transferred for the control volume i, and U is the heat transfer coefficient. T_j, A_j and h_j are the temperatures, areas and enthalpies for the control volume j, respectively. T_h is the ambient temperature.

The ammonia liquid and vapor holdups in the different condenser sections is given by:

$$N_l = \begin{pmatrix} 0 \\ 0.5 \cdot A_2 \\ A_3/3 \\ A_3/3 \\ A_3/3 \end{pmatrix} \cdot \frac{V_{con,tot}}{A_{con,tot}} \rho_l \qquad N_v = \begin{pmatrix} A_1 \\ 0.5 \cdot A_2 \\ 0 \\ 0 \\ 0 \end{pmatrix} \cdot \frac{V_{con,tot}}{A_{con,tot}} \rho_v \tag{4.12}$$

Where A_i is the heat exchange area of section i and N_l, N_v, ρ_l, ρ_v, $A_{con,tot}$, $V_{con,tot}$ are the liquid holdup vector, vapour holdup vector, the liquid and vapour density, the total heat exchange area and the total heat exchange volume, respectively. For these equations it is assumed that the vapour to liquid ratio in the two phase section is 1:1.

The valve

The valve model has the following mathematical relation:

$$\dot{n} = z C_v \sqrt{\rho_l \left(P_h - P_l\right)} \tag{4.13}$$

Here $\dot{n}$ is the flow rate, z the valve opening, C_v the valve constant and P_h, P_l the high and low pressure level, respectively. The valve is assumed to be isenthalp, i.e. the enthalpies at the entrance and the exit are assumed to be the same:

$$h_7 = h_6 \tag{4.14}$$

The evaporator

The evaporator is designed as a cross flow heat exchanger. The energy balance is:

$$Q_{vap} = U A \left(T_c - T_8\right) = \dot{n}(h_{12} - h_7) \tag{4.15}$$

The material balances are:

$$N_l = V_l \rho_l \tag{4.16}$$

$$N_v = V_v \rho_v \tag{4.17}$$

With T_c as the cool room temperature, V_l and V_v the liquid and vapour volumes, respectively.

4.3 The augmented model

As the goal of this work is to introduce internal heat exchange and to find optimal design and subsequently optimal operation with the augmented model, this section deals with introducing internal heat exchange and finding optimal design and operation parameters.

The internal heat exchanger is placed between the condenser and the valve on the high pressure level and between the evaporator and the compresser on the low pressure level. A schematic illustration of the augmented model with the corresponding pressure-enthalpy diagram is shown in figure 4.3.

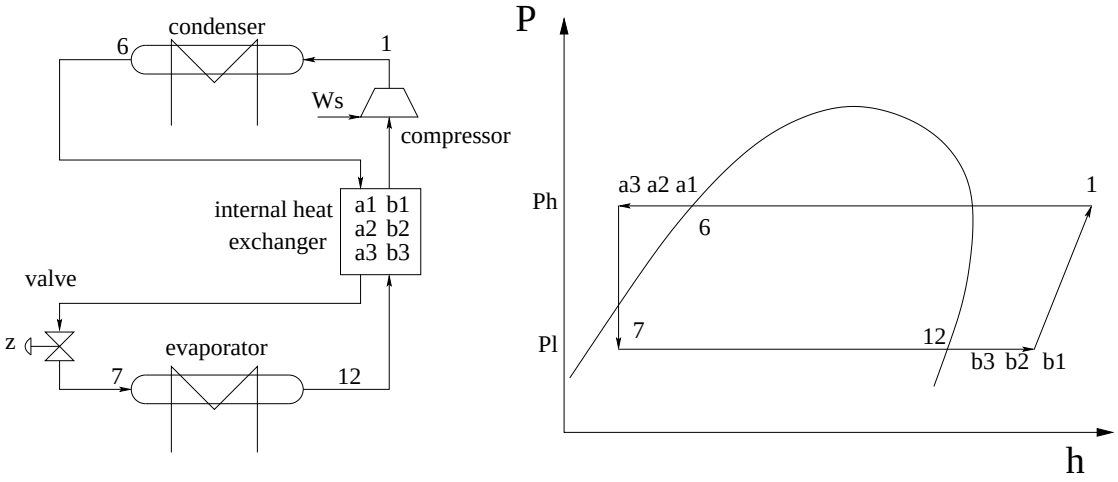

Figure 4.3: System with internal heat exchanger and corresponding P-h-diagram

In the augmented model, again a flooded evaporator is used, so the temperature T_{12} in point 12 is the same as T_7. All superheating is done by the internal heat exchanger. After leaving the condenser with the temperature T_6 the coolant enters the internal heat exchanger and is cooled down to Ta_3 while heating up the vapour to Tb_1. As indicated in the figure, a counterflow heat exchanger is utilized.

4.3.1 Model equations

The equations and the modelling assumptions for the simple model are still valid for the augmented model. In addition it is assumed, that there is no phase change within the internal heat exchanger. As indicated in the figure 4.3, the internal heat exchanger is subdivided into three control volumes. Q_i is the heat exchanged between the control volumes, U and A are the heat transfer coefficient and the heat transfer area. Ta_i and Tb_i are the temperatures of the hot stream a and the cold stream b in the control volumes i.

The heat flows from stream a to stream b:

$$Q_1 = \frac{UA_{ihx}}{3}(Ta_1 - Tb_1) \tag{4.18}$$

$$Q_2 = \frac{UA_{ihx}}{3}(Ta_2 - Tb_2) \tag{4.19}$$

$$Q_3 = \frac{UA_{ihx}}{3}(Ta_3 - Tb_3) \tag{4.20}$$

Here U denotes the heat transfer coefficient and A_{ihx} the total heat exchange area in the internal heat exchanger.

With the flow rate $\dot{n}$, the liquid heat capacity $c_{p,l}$ and the gas heat capacity $c_{p,g}$, the enthalpy changes over the control volumes for the hot stream a and the cold stream b are calculated:

$$Q_1 = \dot{n}c_{p,l}(Ta_{in} - Ta_1) = \dot{n}c_{p,g}(Tb_1 - Tb_2) \tag{4.21}$$

$$Q_2 = \dot{n}c_{p,l}(Ta_1 - Ta_2) = \dot{n}c_{p,g}(Tb_2 - Tb_3) \tag{4.22}$$

$$Q_3 = \dot{n}c_{p,l}(Ta_2 - Ta_3) = \dot{n}c_{p,g}(Tb_3 - Tb_{in}) \tag{4.23}$$

Ta_{in} and Tb_{out} are the temperatures into and out of the internal heat exchanger.

The holdup vectors Na and Nb for the internal heat exchanger are given by following equations:

$$Na = \begin{pmatrix} V_{ihx_a}/3 \\ V_{ihx_a}/3 \\ V_{ihx_a}/3 \end{pmatrix} \cdot \rho_l \qquad Nb = \begin{pmatrix} V_{ihx_b}/3 \\ V_{ihx_b}/3 \\ V_{ihx_b}/3 \end{pmatrix} \cdot \rho_v \tag{4.24}$$

The volumes of the internal heat exchanger V_{ihx_a} and V_{ihx_b} are set equal in this model.

5 Results

5.1 Optimal design

For finding optimal design, first an environment has to be defined. In this work, the design conditions for a large refrigeration system are: Room temperature $T_{c,design} = -12°$ C, outside temperature $T_{h,design} = 25°$ C and the cooling duty $Q_c = 20$ kW. The cost function to be minimized in this thesis is the compressor work $J = W_s$.

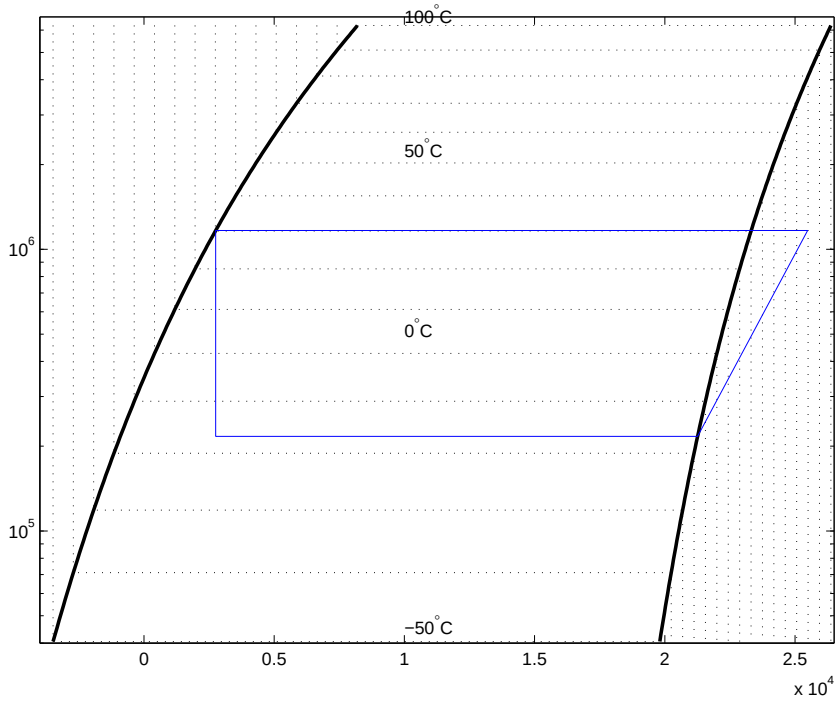

Figure 5.1: P-h-diagram for optimal design (Pressure in [Pa], enthalpy in [W/mol])

In order to find optimal design for this model the cost function J is minimized subject to linear and non linear constraints. The linear constraints are the temperature difference in all heat exchangers:

$$\Delta T_{min} = 5\,\mathrm{K} \tag{5.1}$$

And the cooling duty:

$$Q_c = 20\,\mathrm{kW} \tag{5.2}$$

The minimum temperature difference ΔT_{min} is a common approach to keep the capital and operating costs in reasonable limits. Finally, the nonlinear constraints for optimization are all model equations as described in chapter 4.

All calculations are done with the program MATLAB 6.5 (Mathworks) in combination with the optimizing tool from TOMLAB (Tomlab Optimization). After optimizing the cost function under these constraints, data for optimal design is obtaind. The numerical results of the complete augmented model are listed in table D.1.

It is found that the heat exchange area A_{ihx} of the internal heat exchanger is 0. Accordingly the temperature does not change within the internal heat exchanger and the heat transferred is is zero, too. For an ammonina cooling system designed this way, internal heat exchange is suboptimal. The shaft work, pressure levels and the coefficient of performance are identically the same as for the simple model. Because internal heat exchange is found to be sub optimal, it will not be used further for examining self-optimizing control properties. Optimizing the model without internal heat exchange

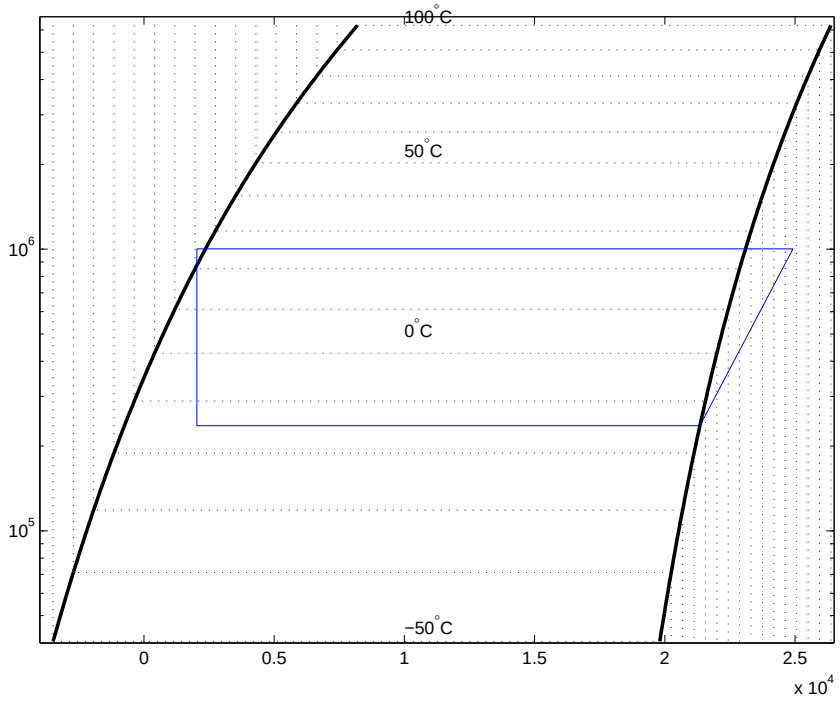

Figure 5.2: Pressure-enthalpy diagram for optimal operation (Pressure in [Pa], enthalpy in [W/mol])

for optimal design, i.e. the same "design" conditions as above, gives the parameter set which is used to study optimal operation. The values are listed in table D.2 in the column "optimal design". The corresponding p-h-diagram is shown in figure 5.1.

5.2 Optimal operation at nominal conditions

For finding optimal operation, the nominal conditions are set differently. The room temperature is $T_{c,op} = -10\,^{\circ}\mathrm{C}$, the outside temperature $T_{h,op} = 20\,^{\circ}\mathrm{C}$. The nominal cooling duty remains $Q_c = 20\,\mathrm{kW}$. Thus, the cooling cycle has been slightly overdesigned.

In optimal operation the inequality constraints $\Delta T_{min} = 5\,\mathrm{K}$ are replaced by equality constraints $A = A_{design}$. The heat exchange area A_{design} is given by design.

The data for optimal operation at nominal conditions are given in table D.2, and the pressure enthalpy diagram is shown in figure 5.2.

5.3 Self-optimizing control

Using the the minimum singular value rule from chapter 2 gives the linear gain for the different variables. The procedure of applying this rule to this specific process is described in appendix A. In this work, only the behaviour of the ideal cycle is considered and the measurement errors and noise are set to zero.

Variable	y_{nom}		Δy	G	$G'(1)$	$G'(2)$
ΔT_{sub}	4.31	[K]	-2.08	-330.69	-20017.26	-39793.65
$N_{l,con,tot}$	956.11	[mol]	-25.26	-4016.48	-157570.75	-244757.99
z	0.63	[-]	0.01	1.00	1250.00	33333.33
$N_{l,vap}$	1899.47	[mol]	23.53	3740.17	-11602.81	-8992.08
$V_{l,vap}$	0.50	[m^3]	0.01	0.983	-12301.27	-8946.38
$\Delta T_{con,end}$	0.69	[K]	1.99	315.64	118216.3	3114.95

Table 5.1: Candidates with high gain for a disturbance of +0.1 K in ambient temperature (1) and +0.05 K in room temperature (2)

Some selected variables with high gain are given in table 5.1. They would be the candidates to keep at a constant setpoint. The linear gain for the other variables is listed in table C.1.

Variable	Disturbance 1 $d = T_c - 5$ K	Disturbance 2 $d = T_c + 5$ K	Disturbance 3 $d = T_h - 10$ K	Disturbance 4 $d = T_h + 10$ K
ΔT_{sub}	0,13	0.69	4.05	0.39
$N_{l,con,tot}$	0.000282	0.000417	0.00311	0.00238
z	12.7	9.75	12.01	10.81
$N_{l,vap}$	0.0086	0.00789	0.03	0.0371
$V_{l,vap}$	0	0.0000134	0.0121	0.0126
$\Delta T_{con,end}$	0.0086	0.00789	0.03	0.0371
P_h	infeasible	2.5	43.3	infeasible
$T_{con,out}$	0.0086	0.0079	infeasible	infeasible

Table 5.2: Additional shaft work W_S (in %) at full disturbance

This linear analysis is only valid at operating points close to the nominal operating

point. To find out whether the candidates are suited for control far from the nominal operating point, it is necessary to check feasibility. This is done by applying full disturbance on the non linear model while holding the variable constant.

The additional shaft work for some selected variables at different disturbances is shown in table 5.2. It can be seen that holding the pressure level P_h and the condenser exit temperature $T_{con,out}$ constant is infeasible for some disturbances. The variables z and the amount of subcooling ΔT_{sub} prove to be poor candidates for constant setpoints. Good candidates are the ones related to the holdups in the condenser and evaporator and the difference between the outside temperature and the condenser exit temperature $\Delta T_{con,end} = T_{con,end} - T_{amb}$.

6 Discussion

6.1 Internal heat exchange

The result of the heat transfer area becoming zero in these calculations can be explained by considering two competing effects of internal heat exchange. It has to be examined, whether internal heat exchange is beneficial or not (Radermacher (1989))

The positive effect of internal heat exchange is that the mixture entering the evaporator has a larger liquid fraction. This means that the same heat can be removed from the cold side using a lower flow rate. As the shaft work is directly proportional to the flowrate, this contributes to a reduction of shaft work.

The negative effect of internal heat exchange is due to the higher compressor inlet temperature. The adiabatic compressor relation $\left(\frac{T_{out}}{T_{in}}\right) = \left(\frac{P_h}{P_l}\right)^{\frac{R}{c_{p,v}}}$ can be introduced into the equation for the compressor work W_s:

$$W_s = \dot{n}c_{p,v}(T_{out} - T_{in}) = \dot{n}c_{p,v}T_{in}\left[\left(\frac{P_h}{P_l}\right)^{\frac{R}{cp,g}} - 1\right] \tag{6.1}$$

From this it is clear that an increased compressor inlet temperature causes increased shaft work.

The calculations in this work show that the effect of the increasing compressor inlet temperature is stronger than the effect of the reduced flow rate. So optimal design for this cycle is without internal heat exchange.

The ratio between $c_{p,l}$ and $c_{p,v}$ seems to be an important factor, as it determines how much the compressor inlet temperature increases (negative effect) compared with the increase in liquid fraction to the evaporator (positive effect). The heat transferred in the internal heat exchanger:

$$Q = UA(\Delta T) = \dot{n}c_{p,l}(T_{liquid,out} - T_{liquid,in}) = \dot{n}c_{p,v}(T_{vapour,out} - T_{vapour,in}) \tag{6.2}$$

For the relation between $c_{p,l}$ and $c_{p,v}$ follows:

$$\frac{c_{p,l}}{c_{p,v}} = \frac{T_{vapour,out} - T_{vapour,in}}{T_{liqudid,out} - T_{liquid,in}} \tag{6.3}$$

As the c_p ratio for this ammonia model is about 1.78, a temperature change on the liquid side of one 1 K results in a change of 1.78 K on the vapour side. This ratio is found to be not optimal for internal heat exchange.

There are, however, ratios of $\frac{c_{p,l}}{c_{p,v}}$ where it is optimal to have internal heat exchange (e.g. a transcritical CO_2-cooling cycle)).

As mentioned before, from a mechanical point of view, a certain amount of superheating is desirable as droplets cause damage in the compressor. So, for a real system of this design, an internal heat exchanger should provide the superheating.

6.2 Optimal design and optimal operation

Comparing the P-h-diagrams for "optimal design" and "optimal operation" it can be seen that there is some subcooling in optimal operation which is not present in in optimal design. This arises because a minimum temperature difference is specified in optimal design. Because a cross flow heat exchanger is used, the pinch is located at the condenser outlet and there is no subcooling. If, however a counter current heat exchanger is used, the pinch point would be located within the condenser, and there would be subcooling in optimal design, too.

In operation there is no specification on the minimum temperature difference and it is possible to find the optimum for the given equipment.

While the coefficient of performance COP has a value of 4.38 for optimal design, it increases about 20 % to 5.41 in operation. As the cooling load is the same for both modes, this is caused by the decreased shaft work.

Because there are no ΔT_{min} requirements in optimal operation, the pressure levels change and subcooling arises. With the pressure ratio decreasing from $\left[\frac{P_h}{P_l}\right]_{des} = 5.37$ to $\left[\frac{P_h}{P_l}\right]_{op} = 4.25$, the compressor work and the flowrate decreases, and the COP rises.

6.3 Self-optimizing control

As mentioned before, the variables related to the holdups in evaporator and condenser prove to be good candidates for self-optimizing control. Keeping the valve at a fixed

setpoint is does not seem to be a good choice for self-optimizing control of an ammonia cycle. It has been found (Jensen and Skogestad (2004)), that in case of a CO_2 cycle the fixed valve strategy is about as good as keeping the evaporator level constant. This hints to that there are some basic differences between subcritical and transcritical cycles.

It is not possible to use P_l as a controlled variable, because the low pressure level is fixed already if the heat flow Q_c and the product of heat transfer coefficient and heat transfer area UA is given.

Keeping P_h at a constant setpoint becomes infeasible for some disturbances. This is because most of the heat is transferred in when the vapor coming from the compressor is condensed at a constant fluid temperature.

If the temperature difference between the fluid and the outside temperature T_h is not high enough for the heat to be removed, operation becomes infeasible. If, however, P_h is free, the transferred heat can be increased by setting the pressure higher. This is not possible, if P_h is kept at a constant setpoint.

Holding the temperature difference between the condenser outlet and the ambient temperature at a constant value is possible, as this strategy sets the temperature at the condenser outlet matching to the disturbance, thus ensuring feasibility.

6.4 Outlook

The step following this work is to introduce implementation errors into the model and to examine how it behaves with respect to self-optimizing control. Possibly also non idealities like valve loss and compressor efficiencies could be taken into account, too. In the course of analyzing the control structure, a dynamic model has to be developed for examination of the control structures. Thereafter more complex processes with mixtures as coolants and with several pressure levels can be considered. Finally cascaded cycles combining all these features can be analyzed and optimized.

A Linear gain for only one manipulated variable

As the minimum singular value of the gain G reduces to the absolute value of the gain $|G|$ in the scalar case, the procedure described in chapter 2.2 is applied to this specific problem as follows:

1. Find the nominal outputs y.
2. Using small disturbances (1% of the expected values) the system is reoptimized to find the change in the states Δy_{opt}.
3. A small step in the independent variable, here the valve opening z, is made. By reoptimizing the change in the outputs Δy is obtained. Thus the linear gain from the independent variable to all outputs can be computed by $G = \frac{\Delta y}{\Delta z}$.
4. Finally the gain is scaled with the optimal changes from step 2 and measurement errors n: $|G'| = \frac{|G|}{|\Delta y_{opt}|+|n|}$

A high value of the absolute scaled gain $|G'|$ is an indication that the variable is a good candidate for a controlled variable c to keep at a constant setpoint c_s.

B Data

The data used for the calculations is listed below.

B.1 Cycle and environment data

$T_{h,des}$	25	°C	Design (hot) ambient temperature
$T_{c,des}$	-12	°C	Design (cold) room temperature
$T_{h,op}$	20	°C	Operation (hot) ambient temperature
$T_{c,op}$	-10	°C	Operation (cold) room temperature
$U_{con,1}$	400	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient in section 1 of condenser
$U_{con,2}$	700	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient in section 2 of condenser
$U_{con,3}$	1000	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient in section 3 of condenser
$U_{con,4}$	1000	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient in section 4 of condenser
$U_{con,5}$	1000	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient in section 5 of condenser
V_{con}	0.5	m^3	Condenser volume
U_{vap}	1000	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient in evaporator
V_{vap}	1	m^3	Evaporator volume
U_{ihx}	300	$\frac{\mathrm{W}}{\mathrm{m^2K}}$	Heat transfer coefficient of the internal heat exchanger
V_{ihx}	0.5	m^3	Internal heat exchanger volume

Table B.1: Cycle and environment data

B.2 Ammonia model data

$c_{p,l}$ $\left[\frac{J}{\mathrm{gK}}\right]$	$c_{p,v}$ $\left[\frac{J}{\mathrm{gK}}\right]$	$\Delta_v h$ $\left[\frac{\mathrm{J}}{\mathrm{g}}\right]$	ρ_l $\left[\frac{\mathrm{g}}{\mathrm{cm}^3}\right]$	T_{ref} [K]	T_{crit} [K]
4.5837	2.5772	1280.57	0.64582	267.79	405.4
A_1	A_4	A_3	A_4	P_c [atm]	
-7.296510	1.618053	-1 956546	-2.114118	111.85	

Table B.2: Fluid model data (from Haar and Gallagher (1978))

C Linear gain analysis

Variable	y_{nom}		Δy	G	$G'(1)$	$G'(2)$
T_{con1}	298.15	[K]	-0.095	-15.05	-126.25	-137.25
T_{con2}	298.15	[K]	-0.095	-15.05	-126.25	-137.25
T_{con3}	295.73	[K]	1.43	226.55	2060.71	2158.08
T_{con4}	294.48	[K]	1.94	308.41	2933.05	3006.83
T_{con5}	293.84	[K]	1.99	315.64	3074.29	3114.95
ΔT_{sub}	4.31	[K]	-2.08	-330.69	-20017.26	-39793.65
$N_{l,con1}$	890.33	[mol]	24.66	3920.73	-17674.48	-34455.84
$N_{l,con2}$	21.93	[mol]	-16.64	-2645.74	-32092.87	-60961.66
$N_{l,con3}$	21.93	[mol]	-16.64	-2645.74	-32092.87	-60961.66
$N_{l,con4}$	21.93	[mol]	-16.64	-2645.74	-32092.87	-60961.66
$N_{l,con,tot}$	956.11	[mol]	-25.26	-4016.48	-157570.75	-244757.99
$N_{v,con1}$	5.28	[mol]	0.05	7.43	207.16	293.014
$N_{v,con2}$	94.78	[mol]	2.37	377.17	1314.09	1378.39
P_h	1002578.18	[Pa]	-2922.12	-464566.08	-125.94	-136.93
z	0.63	[-]	0.01	1.00	1250.00	33333.33
n	1.04	[mol/s]	0.01	1.33	338.65	647.56
T_{vap}	258.15	[K]	0.00	0.00	0.00	0.00
$N_{l,vap}$	1899.47	[mol]	23.53	3740.17	-11602.81	-8992.08
$N_{v,vap}$	554.00	[mol]	-0.68	-108.29	4160.36	-1077.34
$V_{l,vap}$	0.50	[m^3]	0.01	0.983	-12301.27	-8946.38
P_l	236093.23	[Pa]	0.00	0.00	0.00	0.00
W_s	3697.67	[J]	21.25	3378.38	126.90	267.23
$T_{comp,in}$	339.67	[K]	-0.19	-29.90	-114.79	-188.53
$\Delta T_{con,end}$	0.69	[K]	1.99	315.64	118216.3	3114.95

Table C.1: Linear analysis for a disturbance of +0.1 K in ambient temperature ($G'(1)$) and +0.05 K in room temperature ($G'(2)$)

D Variable values

D.1 Augmented model

Variable	Unit	Optimal design
Temperatures:		
T_1	[°C]	79.4
T_2	[°C]	30
T_3	[°C]	30
T_4	[°C]	30
T_5	[°C]	30
T_6	[°C]	30
T_7	[°C]	-17
Ta_1	[°C]	30
Ta_2	[°C]	30
Ta_3	[°C]	30
Tb_1	[°C]	-17
Tb_2	[°C]	-17
Tb_3	[°C]	-17
Condenser holdups:		
$N_{l,2}$	[mol]	921
$N_{l,3}$	[mol]	0
$N_{l,4}$	[mol]	0
$N_{l,5}$	[mol]	0
$N_{v,1}$	[mol]	6
$N_{v,2}$	[mol]	112
Internal heat exchange holdups:		
Na_1	[mol]	633.16
Na_2	[mol]	633.16
Na_3	[mol]	633.16
Nb_1	[mol]	16.96
Nb_2	[mol]	16.96
Nb_3	[mol]	16.96

Augmented model

Variable	Unit	Optimal design
Evaporator holdups:		
$N_{l,vap}$	[mol]	1899
$N_{v,vap}$	[mol]	51
Total holdup:		
N_{tot}	[mol]	4941
Heat transfer in condenser:		
Q_1	[W]	-2339
Q_2	[W]	-22226
Q_3	[W]	0
Q_4	[W]	0
Q_5	[W]	0
Q_{tot}	[W]	-24565
Heat transfer in internal heat exchanger:		
$Q_{ihx,1}$	[W]	0
$Q_{ihx,2}$	[W]	0
$Q_{ihx,3}$	[W]	0
$Q_{ihx,total}$	[W]	0
Heat transfer in evaporator:		
Q	[W]	20000
Heat transfer area in condenser:		
A_1	[m^2]	0.2
A_2	[m^2]	6.35
A_3	[m^2]	0
A_4	[m^2]	0
A_5	[m^2]	0
A_{tot}	[m^2]	6.55
Heat transfer area in evaporator:		
A	[m^2]	4
Heat transfer area in internal heat exchanger:		
A_{ihx}	[m^2]	0

Augmented model

Variable	Unit	Optimal design
Miscellaneus:		
$\dot{n}$	[mol/s]	1.0808
z	[-]	0.5903
W_s	[W]	4565
P_h	[bar]	11.67
P_l	[bar]	2.17
ΔT_{sub}	[K]	0
$\Delta T_{min,con}$	[K]	5
$\Delta T_{min,vap}$	[K]	5
COP_C	[-]	4.38
$V_{l,vap}$	[m^3]	0.5

Table D.1: Variable values for optimal design of the augmented model

D.2 Simple model

Variable	Unit	Optimal design	Optimal operation
Temperatures:			
T_1	[°C]	79.4	66.52
T_2	[°C]	30	25
T_3	[°C]	30	25
T_4	[°C]	30	22.58
T_5	[°C]	30	21.33
T_6	[°C]	30	20.6
T_7	[°C]	-17	-15
Condenser holdups:			
$N_{l,2}$	[mol]	9212	8903
$N_{l,3}$	[mol]	0	219
$N_{l,4}$	[mol]	0	219
$N_{l,5}$	[mol]	0	219
$N_{v,1}$	[mol]	6	5
$N_{v,2}$	[mol]	112	95
Evaporator holdups:			
$N_{l,vap}$	[mol]	18995	18995
$N_{v,vap}$	[mol]	51	55
Total holdup:			
N_{tot}	[mol]	28376	28711
Heat transfer in condenser:			
Q_1	[W]	-2339	-1883
Q_2	[W]	-22226	-21467
Q_3	[W]	0	-195
Q_4	[W]	0	-101
Q_5	[W]	0	-52
Q_{tot}	[W]	-24565	-23698
Heat transfer in evaporator:			
Q	[W]	20000	20000

Simple model

Variable	Unit	optimal design	optimal operation
Heat transfer area in condenser:			
A_1	[m^2]	0.2	0.18
A_2	[m^2]	6.35	6.14
A_3	[m^2]	0	0.08
A_4	[m^2]	0	0.08
A_5	[m^2]	0	0.08
A_{tot}	[m^2]	6.55	6.55
Heat transfer area in evaporator:			
A	[m^2]	4	4
Miscellaneus:			
Flow	[mol/s]	1.0808	1.0353
z	[-]	0.5903	0.6294
W_s	[W]	4565	3698
P_h	[bar]	11.67	10.03
P_l	[bar]	2.17	2.36
ΔT_{sub}	[K]	0	4.31
$\Delta T_{min,con}$	[K]	5	0.69
$\Delta T_{min,vap}$	[K]	5	5
COP	[-]	4.38	5.41
$V_{l,vap}$	[m^3]	0.5	0.5

Table D.2: Variable values for optimal design and optimal operation for the simple model

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