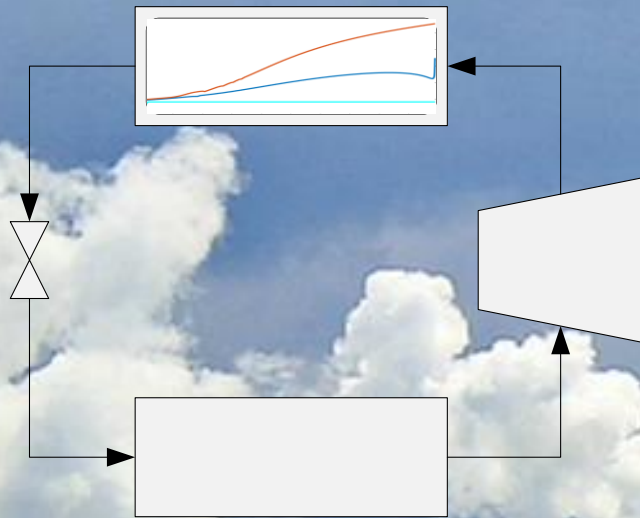


Entropy production minimisation of a compression-resorption heat pump

To save energy and costs in waste heat recovery in industry

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Stefan Aarts
Delft, November 2016

Summary

Waste heat recovery is essential to reduce energy consumption in industry. A heat pump can be used to upgrade waste heat to a temperature level that is suitable for process heat. This study concerns a compression-resorption heat pump. The goal is to optimise the heat pump energetically, while keeping the investment attractive. Entropy production is a measure for energy dissipation and therefore this will be used to quantify the exergetic losses of the cycle. To minimise entropy production is equivalent to optimising the energetic performance.

A literature study is performed and two models are developed and applied to an example case from industry. The first model is used to obtain the coefficient of performance (*COP*) of the cycle and the distribution of the entropy production among the components of the system. The second model can be used to determine the required heat transfer area of the resorber and the distribution of the entropy production inside this component. Both models are used together to make an economical assessment of the system. Also new concepts to improve the heat exchanging process are investigated.

The literature study provides the two following practical notions. The local entropy production rate in process equipment should be equipartitioned to obtain the highest energetic performance. And, to install few large heat exchangers is always a cheaper option than many small ones.

The cycle performance model is developed to assess the energetic performance of the system. This is represented by the coefficient of performance. For the example case the calculations showed that the *COP* can be increased by 26 % with respect to the currently installed pentane vapour-compression heat pump. The optimal concentration of the working fluid is selected. For the example case this concentration is 70 % of ammonia in an ammonia-water mixture. Also, the component with most losses is identified. In the example case this appeared to be the resorber. This is due to the poor match of the temperature profiles in the heat exchanger.

A detailed model is constructed of the resorber. This model provides insight into the process in the plate heat exchanger. The local entropy production is determined using the theory of non-equilibrium thermodynamics. The model suggests that most of the entropy production occurs in the first half of the process.

Together the models are used to evaluate the economic performance of the system at different minimum temperature differences in the resorber. Increasing this temperature difference causes the entropy production, and thus the energy cost of the system to rise, whereas the investment cost is decreased. To reduce the payback period of the system new configurations of the heat exchanging process in the resorber are investigated using the criterion of equipartition of entropy production. These investigations show that distributing the inlet mass flow over the length of the heat exchanger does not decrease the required heat transfer area. Decreasing the cross-sectional area for the flow however, does cause a reduction of the heat transfer area.

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Chapter 1

Introduction

In October 2014 the European Council [12] adopted a climate and energy policy framework for 2030. One of the targets agreed upon was to improve energy efficiency by 27 % compared to projected values based on criteria at that time. In Europe a quarter of final energy consumption is converted in industry [1], so a systematic improvement will have large impact there. One of the ways of systematically improving the efficiency of energy conversion in industry is to use a heat pump to upgrade waste heat to a higher temperature in order to re-use the heat. One method is to apply this system in industry when feasible, and another is to optimise the heat pump itself to gain even greater benefit. The second option is the main topic of this thesis; the optimisation of the performance of such a heat pump. Also a feasibility study will be performed on a specific application in industry. A compression-resorption heat pump (CRHP) is studied. A compression-resorption heat pump is a heat pump that uses a mixture as working fluid. The main advantage and reason for the selection of this type of heat pump is the possibility of increased performance, compared to the well known vapour-compression cycle, depending on the application [7]. The energetic performance of the heat pump is limited in several ways. Physical limits provide knowledge about theoretical opportunity for improvement. And an economic limit indicates to which extent energetic improvements are acceptable for an application.

Objective and strategy

The objective of this thesis is to find the most energy efficient performance for a compression-resorption heat pump keeping the payback time under three years. The energetic performance is defined by the thermodynamic coefficient of performance. A payback time of three years is chosen to ensure an attractive outcome. To achieve this objective first a literature study is performed to increase the understanding of compression-resorption heat pumps, entropy production determination and entropy production minimisation. In order to locate the irreversibilities in the system an entropy production analysis of the cycle is performed. This entails that a model is developed to predict the rate of entropy production in a CRHP. The model is also applied to an example case from industry. The optimal concentration of the working fluid will be selected that causes the least entropy production in the system. The component of the cycle with the most losses will be selected and modelled in detail. The theory of non-equilibrium thermodynamics will be applied to find the distribution of entropy production in that component. Measures to reduce the cost of the component are proposed with the optimality criterion of equipartition of entropy production. This is done by relating the degree of non-ideality to operating conditions and physical characteristics of the system. Also an economic optimisation is performed. This consists of a study that compares investment costs with operating costs of the system in different circumstances. Figure 1.1 shows a schematic diagram of this strategy.

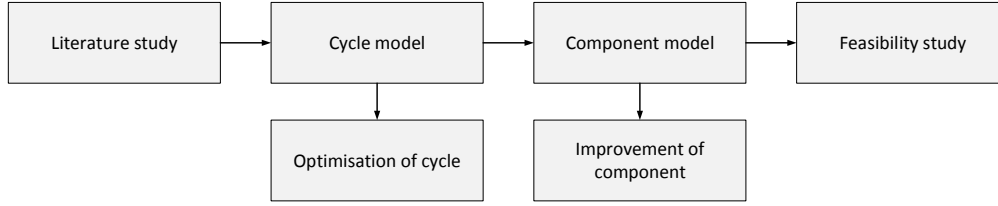


Figure 1.1: Schematic diagram of the strategy to achieve the goal of this thesis.

Application

The application that will be used as example to demonstrate the models that are developed is the supply of heat to a high temperature water heat pump. A water stream of 7.59 kg/s should be heated by the resorber from 89.9°C and 1.1 bar to saturated steam at 104°C . This results in a resorber power demand of 17.5 MW . In the desorber a waste heat stream of dodecane is cooled from 137°C to 40°C . The required mass and heat flow of the source stream depend on the performance of the compression-resorption heat pump. They will become larger as the performance of the heat pump increases. These data are shown in figure 1.2.

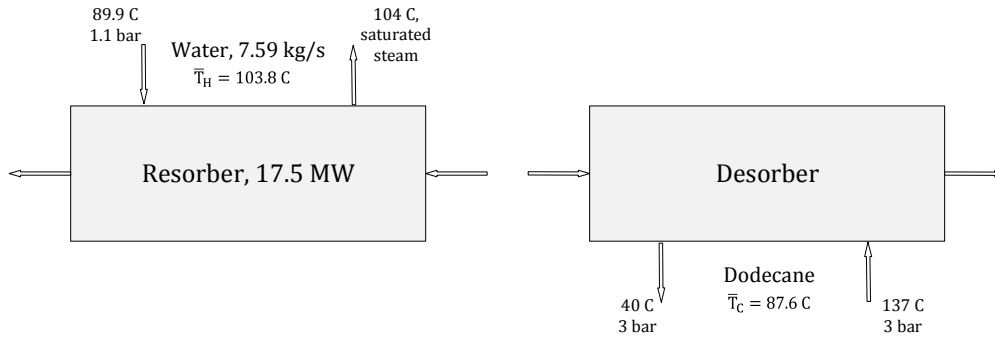


Figure 1.2: Source and sink fluid data of the application that are used as input for the model.

Report structure

In *chapter 2* a theoretical background is given concerning compression-resorption heat pumps and modelling of losses in a thermodynamic system. A model for the calculation of entropy production in the heat pump cycle is presented in *chapter 3*. The model is applied to the example case from industry. This chapter ends with selecting the resorber as the worst performing component of the cycle and an optimisation of the concentration of the working fluid. *Chapter 4* proceeds with detailed model of the resorber. This model gives insight in the internal process in the heat exchanger. The theory of non-equilibrium thermodynamics is applied to obtain the local entropy production in the resorber. In *chapter 5* a feasibility study is performed to show the economical aspects of the application. Then the notion of equipartition of entropy production is used to minimise the resorber area, since there are no degrees of freedom to change its total entropy production. The study ends with conclusions and recommendations for further research in *chapter 6*.

Chapter 2

Theoretical background

In this chapter some topics and principles that are relevant for the study about performance improvement of compression-resorption heat pumps are treated using available literature. The CRHP is explained with its advantages and disadvantages. Then some theory about limits of the performance of such a heat pump is considered. Afterwards the concept of entropy production will be dealt with. Different methods to determine this quantity are presented. Lastly, a principle for an optimal configuration of heat exchangers is derived from an economical perspective.

2.1 Compression-resorption heat pumps

A compression-resorption heat pump is a heat pump that uses a mixture as working fluid. The thermodynamic cycle is a combination of the well known vapour-compression cycle and absorption cycle [2] and it is shown in figure 2.1. The cycle consists of a compressor, resorber, desorber and a valve. Heat enters the cycle from a heat source (in industry often waste heat) into the desorber, work is performed by the compressor and heat is extracted from the cycle via the resorber to a heat sink (an application). A characteristic profile of such a cycle in a temperature-entropy diagram is depicted in figure 2.2.

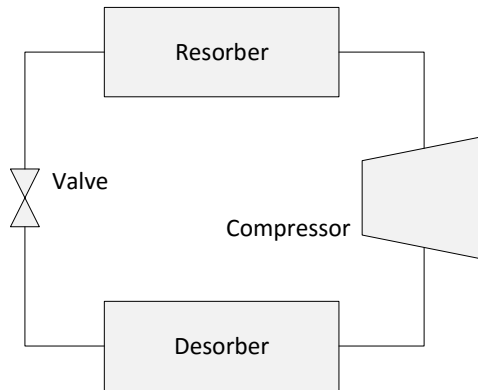


Figure 2.1: Schematic representation of a wet compression-resorption heat pump.

There are different ways to arrange a compression-resorption cycle. In a wet compression-resorption cycle the mixture that leaves the desorber, which is in part still a liquid, is compressed directly by a suitable compressor. On the other hand, in a dry compression-resorption cycle the liquid is separated from the vapour first and then pumped to a higher pressure with a solution pump, while the vapour is compressed by a compressor. Every possible intermediate stage between these two types of cycles can be selected [19].

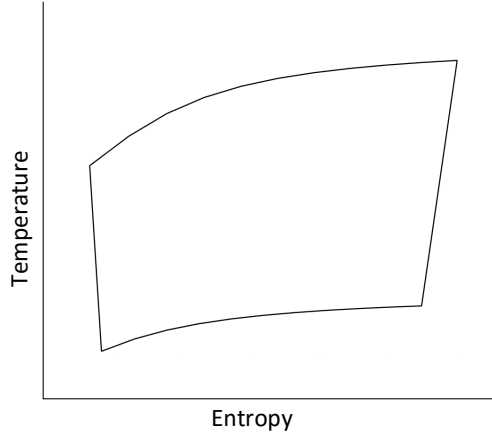


Figure 2.2: Characteristic temperature-entropy diagram for a wet compression-resorption heat pump.

There are several advantages of a compression-resorption cycle compared to a vapour-compression cycle [19, 27, 43].

- The possibility of increased system performance. The temperature profiles of the working fluid are not constant as in a vapour-compression heat pump with a pure working fluid. In a lot of cases the temperature glides fit better to the temperature profiles of the application. Especially when the application is a single phase fluid with a temperature glide. Moreover, the temperature profiles of the working fluid can be adjusted to fit the source and sink temperature profiles by changing the concentration of the mixture. Smaller temperature differences as driving force imply less irreversible heat transfer, so less lost work.
- Reduced saturation pressure of the working fluid, which enables applications at higher temperature. At identical temperature levels the process pressure levels are reduced, this may result in increased compressor life-time.
- The ability to change the temperature profiles by changing the concentration of the mixture. This can be regarded as an additional way to control the capacity of the heat pump.

The impact of these advantages depend on the mixture that is used as a working fluid. For an ammonia-water mixture, which is a commonly used working fluid for compression-resorption heat pumps, these advantages are significant. *COP* improvements are in the range of 4-30 % for various applications (dairy industry, utility buildings and steam production), according to Zaytsev [43]. Van de Bor et al. [7] indicate gains of more than 20 % for industrial applications.

Rijpkema [33] justly mentioned that a disadvantage of fitted temperature profiles is that the driving force for heat transfer is small so that a large heat transfer area is required. This will cause the equipment investment costs to be high.

Challenges that must be faced have to do with the compressor performance. Hulten and Berntson [17] stated that it is not likely that the compressor efficiencies that Itard [19] based her results on (75 %) are feasible. Zaytsev [43] mentioned that the isentropic efficiency of the compressor should be at least 75 % to keep reasonable advantages of the wet compression cycle. The results of his experiments at best only reached 6.6 % however. Infante Ferreira et al. [18] used liquid injection which resulted in an experimental isentropic efficiency of 35 %, and they suggested that a change of mass flow could cause an increase to 50 %.

2.2 Performance limits

It is very useful when considering a thermodynamic system to analyse the theoretical and practical performance limits. These limits provide yardsticks that give a good perspective to the value of the actual performance of the system. Two theoretical performance limits can be derived from the first and second law of thermodynamics.

First law

The first law of thermodynamics for a closed system at steady state can be written as:

$$\dot{Q} + \dot{W} = 0 \quad (2.1)$$

$\dot{Q}$ represents the rate of heat transfer and $\dot{W}$ the rate of work. Both are defined positive when they enter the heat pump system. In a heat pump $\dot{Q} = \dot{Q}_C + \dot{Q}_H$, where $\dot{Q}_C$ is positive and $\dot{Q}_H$ is negative. The subscripts C and H denote the cold side (source) and hot side (sink) of the heat pump respectively. And the COP of a compression-resorption heat pump is the resorber duty divided by the work requirement.

$$COP = \frac{\dot{Q}_H}{\dot{W}} \quad (2.2)$$

For a given application the duty, $\dot{Q}_H$, is fixed. The source heat requirement, $\dot{Q}_C$, can be derived from equation (2.1) and (2.2).

$$\dot{Q}_C = \left(1 - \frac{1}{COP}\right) \dot{Q}_H \quad (2.3)$$

This equation shows the influence of the COP on the source heat. As the COP is increased the source heat is increased as well. When the available waste heat is limited and the resorber duty is fixed the COP of the heat pump is limited. This limit can be calculated when the source and sink heat are known.

$$COP = \frac{\dot{Q}_H}{\dot{Q}_H - \dot{Q}_C} \quad (2.4)$$

From CRHP cycle properties it may be that a higher COP can be achieved. To operate the more efficient cycle one or both of the following alternatives must be executed.

- The available source heat should be increased.
- The duty of the heat pump should be decreased. This means that the CRHP will not complete the task of providing enough heat to the application.

It is important to know for a certain case if one of these measures is acceptable, because if not, the COP is limited by the result of equation (2.4). Fortunately, for the example case that is researched in this work the first alternative is acceptable.

Second law

The second law of thermodynamics can be stated in different ways. The Clausius statement is relevant for heat pumps as it asserts that: *It is impossible for any system to operate in such a way that the sole result would be an energy transfer by heat from a cooler to a hotter body* [26]. This statement implies that it is impossible to operate a heat pump without consuming work.

$$\dot{W} > 0 \quad (2.5)$$

This leads to the notion that the COP of a heat pump must be a finite number. For a reversible (Carnot) heat pump the COP can be determined using the Kelvin scale [26].

$$\left(\frac{\dot{Q}_C}{\dot{Q}_H}\right)_{rev} = \frac{T_C}{T_H} \quad (2.6)$$

The symbol T denotes temperature. Now equation (2.6) can be substituted in the relation for the COP (2.4)

$$COP_{rev} = \frac{T_H}{T_H - T_C} \quad (2.7)$$

This is the equation for the COP of a Carnot cycle which provides the coefficient of performance for an ideal cycle. It only depends on the temperatures of the source and sink of the cycle, and not on the internal system properties, such as refrigerant or capacity. This is the upper performance limit for a heat pump according to the second law, because when irreversibilities are introduced into the system the performance decreases. Theoretically the thermodynamic averaged source and sink temperatures of the surroundings ($\bar{T}_C, \bar{T}_H$) should be regarded when a reversible cycle is considered. Then the COP of a Carnot cycle is not different for heat pumps operating with a mixture instead of a pure component. The thermodynamic averaged temperature of the source can be calculated with:

$$\bar{T}_C = \frac{\Delta h_C}{\Delta s_C} \quad (2.8)$$

This is derived from the second Tds equation on unit mass basis, $Tds = dh - vdp$ [26], where dp is assumed to be negligible in a heat exchanger. The same equation can be used for $\bar{T}_H$ replacing the subscripts C by H . For compression-resorption heat pumps the actual COP is approximately half of the COP of a Carnot cycle; the second-law efficiency is around 50 % [6]. The COP of a Carnot cycle for the application that is considered in this study is 23.3.

In practice there are always irreversibilities present in the system and its surroundings. To minimise them is the task of the engineer and the goal of this study. This minimisation may be limited at last by economic constraints, such as a payback time or a budget.

2.3 Entropy production

Entropy production is a measure of the effect of irreversibilities in a system. It is the most fundamental measure of energy-dissipation [21]. For continuous systems it is the *rate* of entropy production as well as *rates* of energy transfer that are relevant. Two approaches to find the entropy production (rate) of a system will be explained. The first one that will be presented is based on the entropy rate balance.

Entropy rate balance

For a closed heat pump system the entropy rate of change is only influenced by heat exchange with the surroundings and internal irreversibilities. The entropy rate balance can be written as [26]:

$$\frac{dS}{dt} = \sum_i \frac{\dot{Q}_i}{T_i} + \dot{\sigma} \quad (2.9)$$

This equation describes the accumulation of entropy per time-step, $\frac{dS}{dt}$, in a closed system. Entropy is transferred to or from the system by heat, from or to the surroundings and entropy is produced in the system by irreversibilities. The subscript i in the heat transfer term indicates the number of a contribution of heat transfer to the system. And for a component of a heat pump (open system) the entropy rate balance for a control volume around the component can be applied [26].

$$\frac{dS}{dt} = \sum_i \frac{\dot{Q}_i}{T_i} + \sum_j \dot{m}_j s_j - \sum_k \dot{m}_k s_k + \dot{\sigma} \quad (2.10)$$

The terms that are added in equation (2.10) with respect to equation (2.9), account for entropy transfer to and from the system by mass transfer; $\dot{m}$ is mass flow and s is specific entropy. In these equations $\dot{\sigma}$ denotes the rate of entropy production. The subscripts j and k indicate the number of a contribution, just like i , as in equation (2.9). For a component operating at steady state ($\frac{dS}{dt} = 0$) the rate of entropy production can be determined by:

$$\dot{\sigma} = \sum_k \dot{m}_k s_k - \sum_j \dot{m}_j s_j - \sum_i \frac{\dot{Q}_i}{T_i} \quad (2.11)$$

The first two terms on the right hand side represent entropy transfer due to mass transfer and the last term is entropy transfer associated with heat transfer to and from the component. In words equation (2.11) says that the entropy production rate in the control volume must be equal to the difference between the rate at which entropy leaves the system minus the entropy rate entering the system. As a simple example in the case of the refrigerant side of an evaporator that has one inlet and one outlet and one source of heat transfer at constant temperature equation (2.11) reduces to:

$$\dot{\sigma} = \dot{m}(s_{out} - s_{in}) - \frac{\dot{Q}_C}{T_{ev}} \quad (2.12)$$

The first term accounts for entropy transfer by mass transfer and the second for entropy transfer due to heat transfer. The rate at which entropy leaves the system is always greater than the rate at which entropy enters the system and the difference between the two is the entropy production rate. In a desorber of a compression-resorption heat pump the temperature at which heat transfer occurs is not constant. The thermodynamic averaged temperature of the temperature glide, $T_{des} = \bar{T}_{ev}$, should then be used instead of T_{ev} . This averaged temperature, $\bar{T}_{ev}$, can be determined using equation (2.8) when the subscripts C are replaced by ev . The difference between these subscripts is that C denotes the source on the application side and ev denotes the source on the refrigerant side. Using this method to determine the entropy produced in a system is in essence the same as executing an exergy destruction analysis of the system. It is actually the opposite, because when entropy is produced, exergy is destroyed. This approach may be called a global way to assess the rate of entropy production of a system. However, it can be given a more local character when a component is divided into smaller control volumes as applied by Türkakar and Okutucu-Özyurt [40] to a micro-scale heat exchanger.

Non-equilibrium thermodynamics

A different approach which may be called a local way of finding the entropy production rate is described by Kjelstrup et al. [21]. It is the theory of non-equilibrium thermodynamics and it digs down to the nature of entropy production. The field was founded by Onsager with his papers in 1931 [30] [31]. He formulated the second law of thermodynamics in terms of the entropy production.

$$\dot{\sigma} = \sum_i J_i X_i \geq 0 \quad (2.13)$$

It is a summation of conjugate flux-force pairs. The fluxes are denoted by J and the forces by X . Each pair represents an irreversible phenomenon in the system. These phenomena are for example heat transfer, mass transfer, friction and chemical reactions. When the forces and the fluxes of irreversible processes are increased, the entropy production is increased. The forces can be expressed as a linear function of the fluxes.

$$X_i = \sum_j R_{ij} J_j \quad (2.14)$$

Here R represents the phenomenological resistivity coefficient. Furthermore the so-called reciprocal relations are expressed as:

$$R_{ij} = R_{ji} \quad (2.15)$$

These resistivity coefficients determine the coupling between the different phenomena. Coupling is the occurrence of a typical force of a certain phenomenon that acts as a driving force of another phenomenon. For example a temperature difference that causes diffusion. In a heat exchanger with single fluid evaporation or condensation the reversible phenomena are heat transfer and friction. For a volume element inside the heat exchanger equation (2.13) can take the form:

$$\dot{\sigma}_V = \underbrace{\mathbf{J}'_q \cdot \nabla \frac{1}{T}}_{\text{Heat transfer}} - \underbrace{\frac{\mathbf{v}}{T} \cdot \nabla p}_{\text{Friction}} \quad (2.16)$$

The bold symbols stand for tensors. The first term represents a heat flux and a thermal driving force. The second term is a velocity, v , driven by a pressure gradient and scaled with the temperature. The entropy production rate per unit of volume is the result, in $\text{W}/\text{m}^3\text{K}$. Equation (2.16) shows that the

gradients of the fluxes determine the rate of entropy production. A high temperature difference can be related to high entropy production, because the temperature difference causes the force to be high. And a high driving force causes a flux to be high. The global entropy production rate may be obtained by integrating over the volume, V , that is considered.

$$\dot{\sigma} = \int_V \dot{\sigma}_V dV \quad (2.17)$$

Equipartition of entropy production

Daniel Tondeur and Eric Kvaalen [39] studied equipartition of entropy production in 1987. They stated that *for a given duty, the best configuration of an exchanger, contactor, or separator is that in which the entropy production rate is most uniformly distributed*. They proceed to show mathematically, using the theory of non-equilibrium thermodynamics, for an example and in general, that the entropy production of an equipartitioned process is always smaller than of an arbitrary process when the size of the equipment and the duration of the process is kept constant. This is expressed as [39]:

$$\frac{\dot{\sigma} - \dot{\sigma}_{eq}}{Vt} > 0 \quad (2.18)$$

Where $\dot{\sigma}_{eq}$ denotes the entropy production of an equipartitioned process and $\dot{\sigma}$ denotes the entropy production rate of an arbitrary process. This is an impressive observation with high potential for benefit in the study of energetic optimisation of process equipment. In this study the resorber of the heat pump cycle will be optimised by considering the uniformity of the distribution of entropy production in the heat exchanger.

2.4 Heat exchanger configuration

When for a certain application the total heat exchanging area is considered to be fixed, a choice can be made for many small heat exchangers or few larger ones. They can be placed either in series or in parallel. All operating conditions are considered to be given for a certain application so the total entropy production is not affected. Therefore, economic arguments can be used to select the right configuration. The operating cost of the system is not changed by the configuration; only the capital cost is. A plate heat exchanger is selected because it is an established heat exchanger type with available design methods and economic data. Also investigations have been made using an ammonia-water mixture by Táboas et al. [38]. The capital cost can be calculated with a method proposed by Sinnott and Towler [37]. For a plate heat exchanger the cost can be calculated with the following correlation.

$$C = 1350 + 180A_{hex}^{0.95} \quad 1 < A_{hex} < 500 \quad (2.19)$$

The heat exchanging area of one heat exchanger (A_{hex}) is the total required heat exchanging area divided by the number of heat exchangers $A = A_{hex}/k$. Knowing that the total heat exchanging area remains the same and adding a factor for the number of heat exchangers the correlation becomes:

$$C = \left(1350 + 180 \left(\frac{A}{k} \right)^{0.95} \right) k \quad 1 < \frac{A}{k} < 500 \quad (2.20)$$

Let the total heat exchanging area of be assumed to be 3000 m². Now the cost of the equipment can be plotted as a function of the number of heat exchangers. This is shown in figure 2.3. From the figure it is clear that fewer and larger heat exchangers are always a cheaper option. Equation (2.19) is only valid for heat exchangers up to 500 m². Plate heat exchangers can be up to 1500 m² [37], but that is exceptional. To keep to a conventional size the number of heat exchangers must therefore not be lower than 6.

When a process of phase change occurs, then it is expected that placing the heat exchangers in series will lead to lower capital costs than placing the parallel to each other. Because the separate heat exchangers can be designed taking the density of the fluid inside into consideration. This is not investigated further.

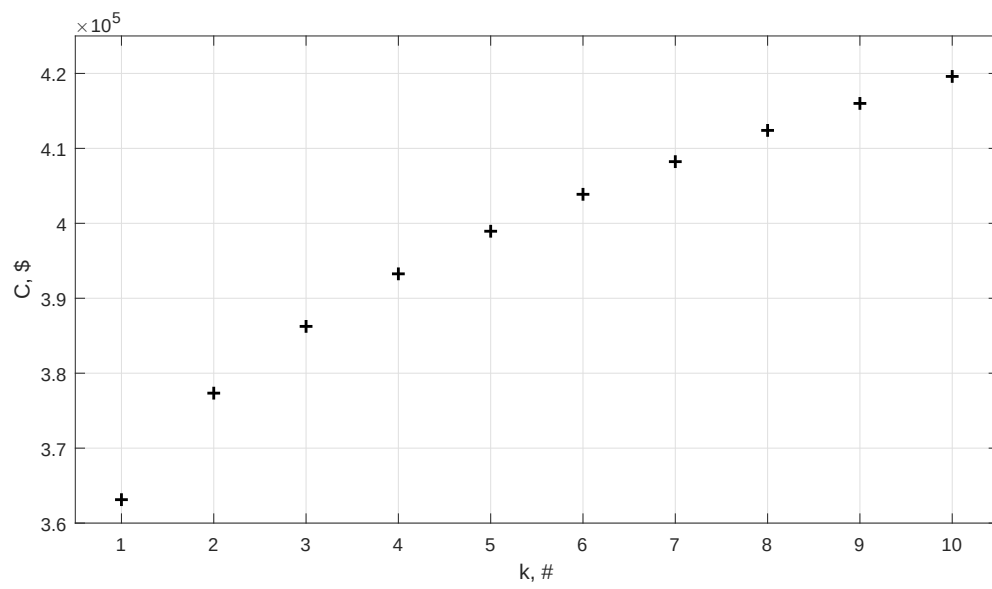


Figure 2.3: Cost of the heat exchanger depending on the number of heat exchangers.

Chapter 3

Cycle performance optimisation

This chapter is concerned with the performance of a compression-resorption heat pump as a cycle. A model is described and then applied to the application that was introduced in *chapter 1*. The optimal concentration is found and the optimal performance of the CRHP is placed in the context of other solutions for the same application. Furthermore, the model can be used to select the component with the highest entropy production for further investigations.

3.1 Model description

A compression-resorption cycle consists of four components; a compressor, a resorber, a desorber and a valve. The entropy production rate of each of these components is determined using the entropy rate balance for a control volume around the component. The entropy production rate can be expressed with equation (2.11). In this section the entropy production rate is determined for each component of the heat pump. The result provides insight into the rate of work that is lost in each component. The components can be compared to each other and the components that dissipate the most energy, and thus require closest attention in an optimisation approach, can be identified. For convenience the entropy production rate derived from the entropy rate balance for an open system is repeated here.

$$\dot{\sigma} = \sum_k \dot{m}_k s_k - \sum_j \dot{m}_j s_j - \sum_i \frac{\dot{Q}_i}{T_i} \quad (3.1)$$

In the simple model treated in this section heat exchange with the environment is ignored, so the last term drops out of equation (3.1). The schematic illustration of a compression-resorption cycle is shown in figure 3.1 to be used as reference for the notation of state points in the equations below.

The entropy production rates deduced from equation (3.1) for each component of the heat pump are written as in equations (3.2)-(3.5). These relations are derived simply by considering all in- and outlet entropy flows of each component and heat losses to the environment are ignored.

$$\text{Compressor} : \dot{\sigma} = \dot{m}_R(s_2 - s_1) \quad (3.2)$$

$$\text{Resorber} : \dot{\sigma} = \dot{m}_R(s_3 - s_2) + \dot{m}_H(s_{H_{out}} - s_{H_{in}}) \quad (3.3)$$

$$\text{Desorber} : \dot{\sigma} = \dot{m}_R(s_1 - s_4) + \dot{m}_C(s_{C_{out}} - s_{C_{in}}) \quad (3.4)$$

$$\text{Valve} : \dot{\sigma} = \dot{m}_R(s_4 - s_3) \quad (3.5)$$

The mass flows and specific entropy values of the source and sink ($\dot{m}_H, \dot{m}_C, s_{H_o}, s_{H_i}, s_{C_i}, s_{C_o}$) are determined by the particular application that the heat pump is integrated in. To obtain the mass flow and the specific entropy values of the working fluid ($\dot{m}_R, s_1, s_2, s_3, s_4$) a working fluid must be selected and cycle calculations must be performed. A commonly used working fluid is a mixture of ammonia and water. For the cycle calculations the approach of van de Bor [6] could be used where state 2 is taken as saturated vapour (highest performance) and then the pressure at state 1 is obtained in an iterative manner. This approach uses the following assumptions.

- No pressure drops in the heat exchangers and pipes

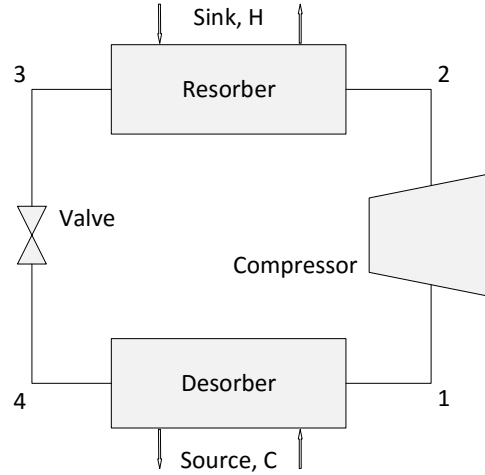


Figure 3.1: Schematic representation of a wet compression-resorption heat pump as shown in figure (2.1) with added notation for reference in this section.

- No heat loss to surroundings
- Isentropic efficiency of the compressor of 70 %
- Minimum temperature difference between the fluids in the heat exchangers is 5 K

The total entropy production is obtained by adding up that of the separate components. Now the lost work of the system may be determined using the Gouy-Stodola theorem [5]:

$$\dot{W}_{lost} = \dot{W} - \dot{W}_{rev} = T_0 \dot{\sigma} \quad (3.6)$$

The entropy production is multiplied by the temperature of the environment T_0 . Another name for the lost work $\dot{W}_{lost}$ is the rate of exergy destruction $\dot{E}_d$. In order to calculate the COP of the system the second law efficiency should be determined by:

$$\eta_{II} = \frac{\dot{W}_{rev}}{\dot{W}} = 1 - \frac{\dot{W}_{lost}}{\dot{W}} \quad (3.7)$$

$\dot{W}$ is the rate of work that is performed by the compressor. Now the COP of the system can be calculated using the COP of a reversible cycle.

$$COP = \eta_{II} COP_{rev} \quad (3.8)$$

The COP of a reversible cycle was previously expressed by equation (2.7).

3.2 Example

The calculation is applied to the application that was introduced in *chapter 1*. For this example the cycle calculations of van de Bor [6] are executed, together with the computation method for properties of ammonia-water of Rattner and Garimella [32], to obtain properties of the working fluid at each state point in the heat pump. Then the entropy production and performance model that has been presented in this section is implemented. The working fluid that is considered is a mixture of ammonia and water. Table 3.1 shows the input conditions and the results. In figure 3.2 a temperature-entropy diagram is shown of the mixture in the compression-resorption heat pump. Figure 3.3 shows the temperature profiles of both fluids in the resorber and the desorber. For low entropy production, low temperature differences are desired; this means that the temperature profiles in a heat exchanger should match each other. The figure shows that there is room for improvement of the temperature profiles.

From the results of the separate rates of entropy production in the components it can be seen that most of the energy dissipation in the heat pump occurs in the resorber (37 %), the compressor (29

Table 3.1: Performance results of the compression-resorption heat pump integrated in the application.

Working fluid: ammonia 30 %, water 70 % (molar)							
η_{is} : 70 %, $T_0 = \bar{T}_C$: 360.7 K, $\dot{m}_R$: 8.15 kg/s							
state	T, K	h, kJ/kg	s, kJ/kg K	$\dot{\sigma}$, kW/K			
1	342.2	1773	6.02	Compressor:	3.60	$\dot{W}_{lost}$	4.47 MW
2	437.3	2413	6.46	Resorber:	4.59	η_{II}	14.5 %
3	377.8	269	1.34	Desorber:	3.05	COP	3.35
4	308.2	269	1.48	Valve:	1.14		
				Total:	12.38		

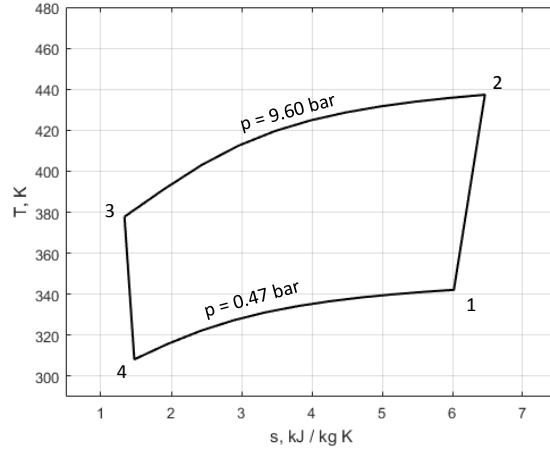


Figure 3.2: Temperature-entropy diagram for the compression-resorption heat pump integrated in the application.

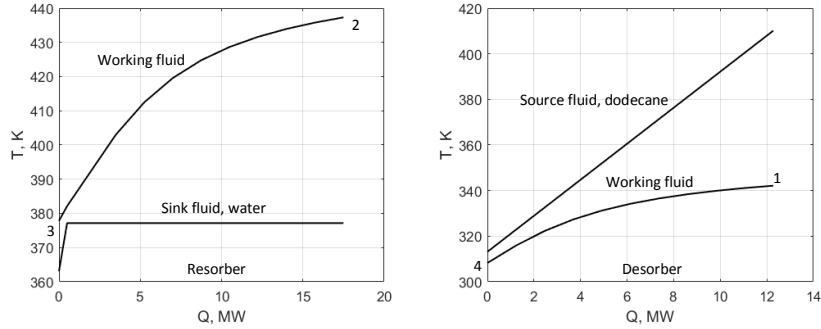


Figure 3.3: Temperature profiles in the resorber (left) and the desorber (right).

%) and the desorber (25 %). These are the components that need closest attention in an optimisation study.

The isentropic efficiency of the compressor is important for an efficient system. If η_{is} were only 60 % instead of 70 % for instance, the COP would decrease to 2.99. In this situation the the distribution of entropy production among the components changes as well. The contributions become 38 % for the compressor, 32 % for the resorber and 21 % for the desorber.

To check the model, the COP may be calculated also in another way. Namely by using the definition of the COP that is given in equation (2.2). It can be worked out as:

$$COP = \frac{\dot{Q}_H}{\dot{W}} = \frac{-(h_3 - h_2)}{h_2 - h_1} = \frac{-(269 - 2413)}{2413 - 1773} = 3.35 \quad (3.9)$$

The outcome is equal to the result of equation (3.8) that is shown in table 3.1.

3.3 Optimisation

The second-law efficiency is only 14.3 % (Table 3.1) and this means that there is relatively much entropy produced. As mentioned in *chapter 2* the second law efficiency of a CRHP is usually around 50 % [6]. The principal reason for this must be the mismatch between the temperature profiles in the heat exchangers. To optimise the performance of the cycle the control variables may be adjusted. For the given application the degrees of freedom are limited. The duty of the resorber is given and the temperature profiles of the source and sink are also fixed. What can be changed is the concentration of the working fluid mixture and the heat exchanger configuration.

To assess the influence of the ammonia concentration on the performance, the model described in this chapter should be executed for different concentrations. Figure 3.4 shows the results of this procedure. The performance seems to be maximal at a concentration around 70 %.

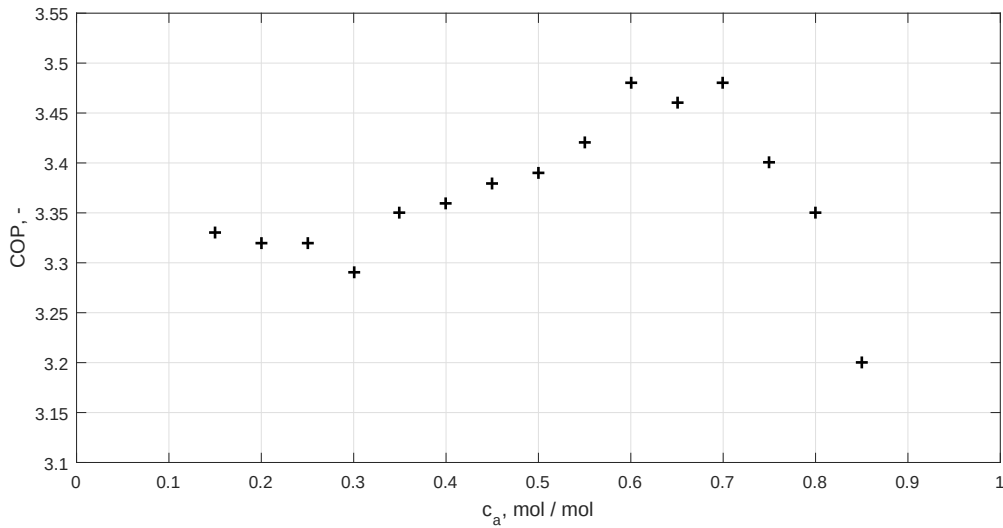


Figure 3.4: Coefficient of performance at different ammonia concentrations.

The model becomes unstable below concentrations of 15 % so calculation was impossible. According to van de Bor [6] the COP rises for ammonia concentrations below 15 % as the concentration decreases. However, the minimal concentration that must be used is 25 % to ensure that the pressure in the compressor is not below 0.3 bar. A lower pressure in the compressor could cause failure. So the optimal concentration is indeed 70 %. The inconsistency of the points is caused by numerical rounding errors.

Table 3.2: Performance results of the compression-resorption heat pump integrated in the application with optimised concentration.

Working fluid: ammonia 70 %, water 30 % (molar)							
η_{is} : 70 %, $T_0 = \bar{T}_C$: 360.7 K, $\dot{m}_R$: 10.69 kg/s							
state	T, K	h, kJ/kg	s, kJ/kg K	$\dot{\sigma}$, kW/K			
1	381.2	1491	4.98	Compressor:	3.24	$\dot{W}_{lost}$	4.28 MW
2	471.3	1961	5.28	Resorber:	5.29	η_{II}	15.0 %
3	379.8	324	1.43	Desorber:	1.58	COP	3.48
4	307.9	324	1.60	Valve:	1.75		
Total:					11.86		

The results of the cycle with the ammonia concentration of 70 % are shown in table 3.2, figure 3.5 and figure 3.6. The second-law efficiency at this concentration becomes $\eta_{II} = 15.0$ %, so there is a small increase with respect to the result of the example above ($\eta_{II} = 14.3\%$) using a concentration

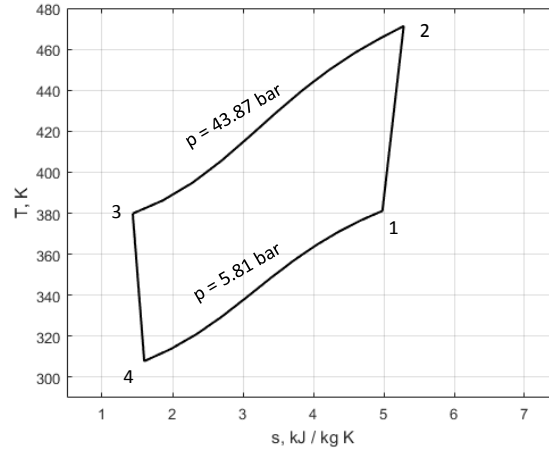


Figure 3.5: Temperature-entropy diagram for the compression-resorption heat pump integrated in the application when the mixture concentration is 70 %.

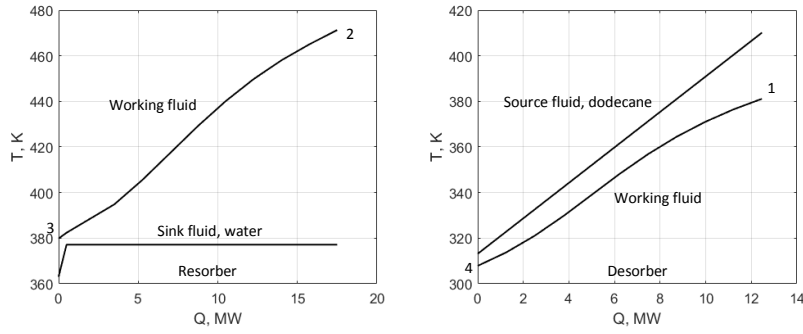


Figure 3.6: Temperature profiles in the resorber (left) and the desorber (right) when the mixture concentration is 70 %.

of 30 %. The temperature profiles change when the concentration of the mixture is different. The new temperature profiles are depicted in figure 3.6. The profiles in the desorber match better at a concentration of 70 % compared to a concentration of 30 %. However, the profiles in the resorber have become worse. Overall there is a small increase in performance; that is indicated by the *COP*.

Context

To have an understanding of the performance of the CRHP for the considered application it is good to put it in the context of other options for the same application. Table 3.3 shows the performance of five different options. Currently a vapour-compression heat pump (VCHP) is installed with a mass flow of the source fluid of 40.0 kg/s. The performance of this heat pump is restricted to the limit of the first law (see equation (2.4)). The performance of the current installation can be increased to 2.76, when the mass flow of the source fluid is increased to 47.1 kg/s. If another working fluid is used in the VCHP, the performance may be increased even further. In appendix A results are shown of performance calculations of different fluids in a VCHP. Acetone has the highest performance from the fluids that have been investigated. The CRHP with an ammonia-water concentration has the highest performance; the relative advantage does not seem very impressive. However, on a large scale small performance improvements have great impact.

Table 3.3: Performance results of different heat pumps integrated in the same application.

Cycle	Working fluid	$\dot{m}_C$, kg/s	COP , -
VCHP	pentane	40.0	2.03
VCHP	pentane	47.1	2.76
CRHP*	ammonia-water, 30 %	49.1	2.99
VCHP	acetone	51.4	3.29
CRHP	ammonia-water, 30 %	51.8	3.35
CRHP	ammonia-water, 70 %	52.6	3.48

* with η_{is} = 60 % instead of 70 %.

Chapter 4

Resorber model

In this chapter a model is presented that is aimed at calculating entropy production of resorption in a plate heat exchanger. This component has been selected to be modelled in detail because in *chapter 3* it was shown that it had the highest entropy production for the considered application. For the development of the entropy production model the approach of Kjelstrup et al. [20] [21] is the basis. In this approach entropy production is governed by irreversibilities, as is the case physically. The heat and mass fluxes are calculated with energy and mass balances, using the strategy of a model that was developed for vertical tubular absorbers by Fernández-Seara et al. [13]. Also temperatures and concentrations of the fluid are calculated in this way. Transfer coefficients are modified to suit the type of flow in a plate heat exchanger, rather than a vertical tubular absorber. First the theory of non-equilibrium thermodynamics will be applied to the case of falling film condensation of a mixture of ammonia-water in a plate heat exchanger to calculate local entropy production. Afterwards a detailed thermodynamic state model of the heat exchanger will be presented that provides the required data for the entropy production calculation.

4.1 Applied non-equilibrium thermodynamics

The entropy production rate will be determined using the theory of non-equilibrium thermodynamics. Falling film condensation of an ammonia-water mixture in a plate heat exchanger is considered. Figure 4.1a shows a condensate film falling down along a plate of a heat exchanger. In filmwise condensation of a mixture irreversibilities are present in the vapour, the liquid film and the interface between them. Also the heat exchanged through the wall and in the cooling medium results in a contribution to the entropy production. The cooling medium of the application is evaporating water. To determine the total entropy production of a control volume the different contributions should all be added up together.

$$\dot{\sigma} = \dot{\sigma}^l + \dot{\sigma}^v + \dot{\sigma}^i + \dot{\sigma}^W + \dot{\sigma}^{cm} \quad (4.1)$$

Irreversible processes that occur are heat transfer, friction and mass transfer. In this chapter friction is neglected, because it is not expected to play an important role in the calculation of the entropy production rate. In the condensate film as well as in the vapour, entropy production may originate from heat transfer and mass transfer [20]. Since there is no concentration gradient in the vapour, nor in the liquid (see figure 4.1c), there is no mass transfer there. Only heat transfer produces entropy and this can be expressed by equation (4.2) for the liquid. The local entropy production is a function of x since the temperature changes along that coordinate, see figure 4.1c.

$$\dot{\sigma}^l(x) = J_q^l \frac{\partial}{\partial x} \left(\frac{1}{T^l(x, y)} \right) \quad (4.2)$$

Integration of $\dot{\sigma}^l(x)$ over the the distance dx yields the total entropy production rate in the liquid region, $\dot{\sigma}^l$, that is suitable for equation (4.1). The distance dx is the film thickness δ_f for the liquid. Equation (4.2) can be used to determine the entropy production in the wall and the cooling medium as well. The superscripts l should then be replaced by W or cm , for wall and cooling medium respectively. There

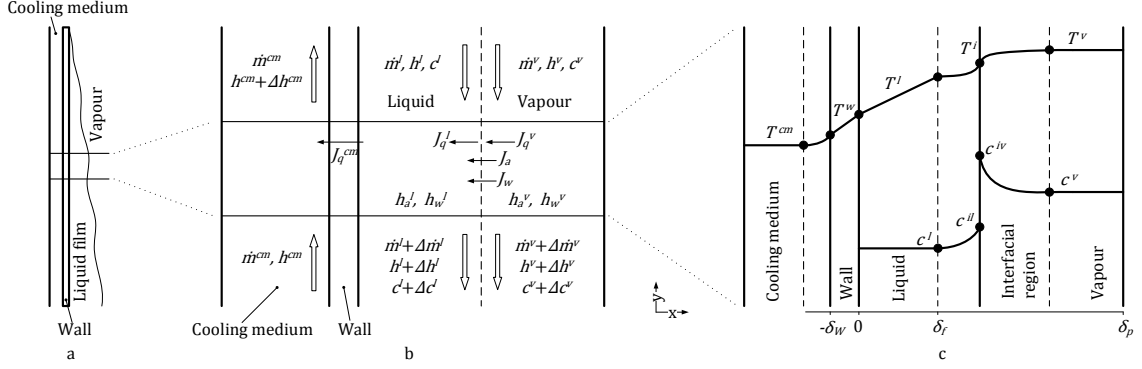


Figure 4.1: Three representations of the condensate film with increased detail from left to right. The arrows define which directions are positive. Parts are modified figures from ref. [13] and [14].

is no entropy production from heat transfer in the vapour, because there is no temperature gradient in the vapour ($\dot{\sigma}^v = 0$). According to Onsager's formulation of the second law, the fluxes are a linear combination of the forces. In this case there is only one flux-force pair, so the flux equation reduces to Fourier's law for the liquid:

$$J_q^l = -\lambda^l \frac{\partial T^l(x, y)}{\partial x} \quad (4.3)$$

The conductivity λ^l of the liquid film is calculated using the method of Conde [11]. The heat flux through the wall J_q^W can be calculated with equation (4.3) as well, with the conductivity of the wall and the temperature gradient in the wall. The heat flux from the wall to the cooling medium is equal to the heat flux through the wall ($J_q^{cm} = J_q^W$). The temperature gradients in the liquid and the wall are constant (see figure 4.1c). They can be estimated with:

$$\frac{\partial T^l}{\partial x} = \frac{T^l(\delta_f, y) - T^l(0, y)}{\delta_f} \quad (4.4)$$

$$\frac{\partial T^W}{\partial x} = \frac{T^W(0, y) - T^W(-\delta_W, y)}{\delta_W} \quad (4.5)$$

The x-coordinates in these equations are also shown at the bottom of figure 4.1c. δ_W is the wall thickness. Although there is evaporation taking place in the cooling medium, the entropy production rate is calculated in the same way as for a single fluid with Fourier's law as a rough approximation. The temperature gradient in the cooling medium is assumed to be zero, except for the liquid boundary layer along the wall. There the temperature profile is assumed to be according to:

$$T^{cm_b}(x, y) = \frac{T^W(-\delta_W, y) - T^{cm}(-(\delta_W + \delta_b), y)}{\delta_b^4} \cdot (x + \delta_W + \delta_b)^4 + T^{cm}(-(\delta_W + \delta_b), y) \quad (4.6)$$

δ_b is the boundary layer thickness which is estimated as $\delta_p/10$; δ_p is the plate spacing. The temperature profile is depicted in figure 4.2. The x-coordinate in figure 4.2 corresponds to that of figure 4.1c and it is displayed in the domain $-(\delta_W + \delta_b) < x < -\delta_W$. The temperature gradient in the boundary layer can be obtained by differentiating equation (4.6).

$$\frac{\partial T^{cm_b}}{\partial x} = \frac{T^{cm_b}(-\delta_W, y) - T^{cm_b}(-(\delta_W + \delta_b), y)}{\delta_b^4} \cdot 4(x + \delta_W + \delta_b)^3 \quad (4.7)$$

The entropy production rate in the interface between the vapour and the liquid is calculated differently, for heat and mass transfer processes are present in the interface.

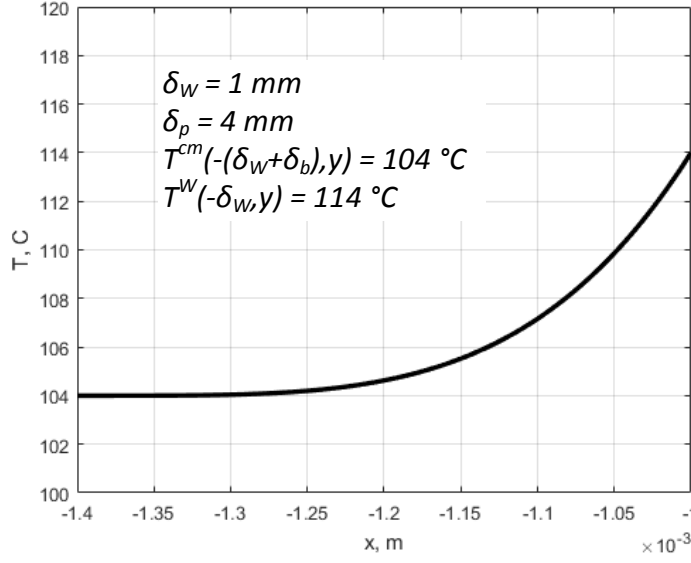


Figure 4.2: Temperature profile of the boundary layer in the cooling medium.

Entropy production rate of the interface

In figure 4.1c the interfacial region is enclosed by the dashed vertical lines on the working fluid side. The entropy production rate in this region is derived by Kjelstrup and Bedeaux [20] to be written as shown in equation (4.8).

$$\dot{\sigma}^i = J_q^v \Delta_{v,l} \left(\frac{1}{T} \right) + J_a \left[-\frac{1}{T^l} \Delta_{v,l} \mu_{a,T}(T^l) \right] + J_w \left[-\frac{1}{T^l} \Delta_{v,l} \mu_{w,T}(T^l) \right] \quad (4.8)$$

Subscript a is used for ammonia, and w for water. And the subscript T indicates that the chemical potentials must be evaluated at constant temperature, T^l . The reason for the evaluation of both chemical potentials at the liquid temperature is a mathematical trick by Kjelstrup and Bedeaux [20], using the Gibbs-Helmholz equation.

Force equations can be now written in terms of resistivities as is elaborated on by Kjelstrup and Bedeaux [20]. Not all resistivities can be determined, because some of them depend on the condensation coefficient. The condensation coefficient is the fraction of molecules in the vapour that are absorbed into the liquid after collision at the interface. This coefficient is unknown for ammonia and somewhat controversial for water [20]. Instead it is suggested to write the forces in terms of temperature differences and concentration differences. And the fluxes are determined with a thermodynamic model based on that of Fernández-Seara et al. [13]. The heat transfer force can be expressed as:

$$\Delta_{v,l} \left(\frac{1}{T} \right) = \frac{1}{T^l} - \frac{1}{T^v} = \frac{T^v - T^l}{T^l T^v} \quad (4.9)$$

And the mass transfer driving forces can be derived using the following definition of the chemical potential.

$$\mu_j = \mu^0 + RT \ln \left(\frac{c_j \phi_j p}{p^*} \right) \quad (4.10)$$

Here R is the universal gas constant. ϕ_j is the partial fugacity coefficient of component j , which can be either ammonia or water. For each component there is a driving force. For ammonia the driving force is the difference in chemical potential between the liquid and the vapour.

$$-\frac{1}{T^l} \Delta_{v,l} \mu_{a,T}(T^l) = -\frac{1}{T^l} \left[\mu^0 + RT^l \ln \left(\frac{c_a \phi_a(T^l) p}{p^*} \right)_l - \left(\mu^0 + RT^l \ln \left(\frac{c_a \phi_a(T^l) p}{p^*} \right)_v \right) \right] \quad (4.11)$$

$$= -R \ln \left(\frac{(c_a \phi_a(T^l))_l}{(c_a \phi_a(T^l))_v} \right)$$

Both partial fugacity coefficients must be evaluated at the liquid temperature. The driving force for water can be derived similarly.

$$-\frac{1}{T^l} \Delta_{v,l} \mu_{w,T}(T^l) = -R \ln \left(\frac{(c_w \phi_w(T^l))_l}{(c_w \phi_w(T^l))_v} \right) \quad (4.12)$$

At constant pressure and constant overall ammonia concentration the fugacity coefficients depend only on the temperature. At $p = 44$ bar and $c_a = 0.7$ mol/mol the partial fugacity coefficients for each phase can be expressed as:

$$\phi_a^l = 1.226 \cdot 10^{-5} T^2 + 5.901 \cdot 10^{-3} T - 2.836 \quad (4.13)$$

$$\phi_a^v = -6.395 \cdot 10^{-6} T^2 + 6.487 \cdot 10^{-3} T - 0.7188 \quad (4.14)$$

$$\phi_w^l = 1.281 \cdot 10^{-7} T^3 - 1.303 \cdot 10^{-4} T^2 + 4.432 \cdot 10^{-2} T - 5.039 \quad (4.15)$$

$$\phi_w^v = 1.222 \cdot 10^{-7} T^3 - 1.686 \cdot 10^{-4} T^2 + 7.961 \cdot 10^{-2} T - 12.112 \quad (4.16)$$

The correlations have been generated based on data from Refprop [24].

In order to have enough information, such as temperatures and concentrations, for calculation of the entropy production, a thermodynamic state model must be developed.

4.2 Thermodynamic state model

In this section an explanation is given of a detailed thermodynamic model of a resorber. In the resorber film condensation of an ammonia-water mixture takes place. This model is used to calculate thermodynamic states and transport processes in the resorber. The model is based on the work of Fernández-Seara et al. [13]. The heat exchanger is divided into a number of cells. In each cell driving forces are used to determine mass and energy fluxes which dictate the progress of the process to the next cell. Figure 4.1b can be helpful to get an impression of which variables and fluxes are important in a cell. Figure 4.3 shows a flow diagram of the iterative loops that are solved for each cell. The two iteration loops are depicted as dashed lines. The large loop is for determining the interface temperature, T^i , with the energy balance over the vapour-liquid interface. The other loop is for determining the ammonia flux ratio, z , with the mass balance over the interface.

First, the two iterative loops to satisfy the energy and mass balance will be explained; they contain the governing equations of the model. Then the inputs and initial values for the loops are dealt with. The inputs are all a result of the application considered. The initial values (T^i and z) must be guessed with some justification. Thirdly, the equations for the next cell are shown; these are crucial for the theoretical behaviour of the substances in the heat exchanger. Then the method is treated to obtain the heat and mass transfer coefficients that are variable along the heat exchanger. These transfer coefficients determine the degree of heat and mass transfer at the different transfer locations.

In the calculations in this section the naming of the temperatures is slightly different than in figure 4.1c. Every dot on the temperature profile in figure 4.1c is a temperature node here. The names that are given to the nodes from right to left are: T^{cm} , T^{Wo} , T^{Wi} , T^l , T^i , T^v . The names of the concentration nodes are used as is indicated in figure 4.1c.

4.2.1 Iterative loops

The model starts with a guess of the interface temperature as is indicated in the flow diagram. Following the large circle in clockwise direction each calculation step will be treated in this section. First the molar concentrations at the interface are determined. For this equilibrium is assumed at the interface according to the two-film theory of Whitman [35]. To obtain the concentration a property call is executed, which requires the interface temperature and the pressure in the resorber.

$$c_a^i = c(T^i, p, q) \quad (4.17)$$

For the liquid the quality, q , is set to 0 and for the vapour to 1. The property calls for the ammonia water mixture are performed with the method of Rattner and Garimella [32]. A molar concentration

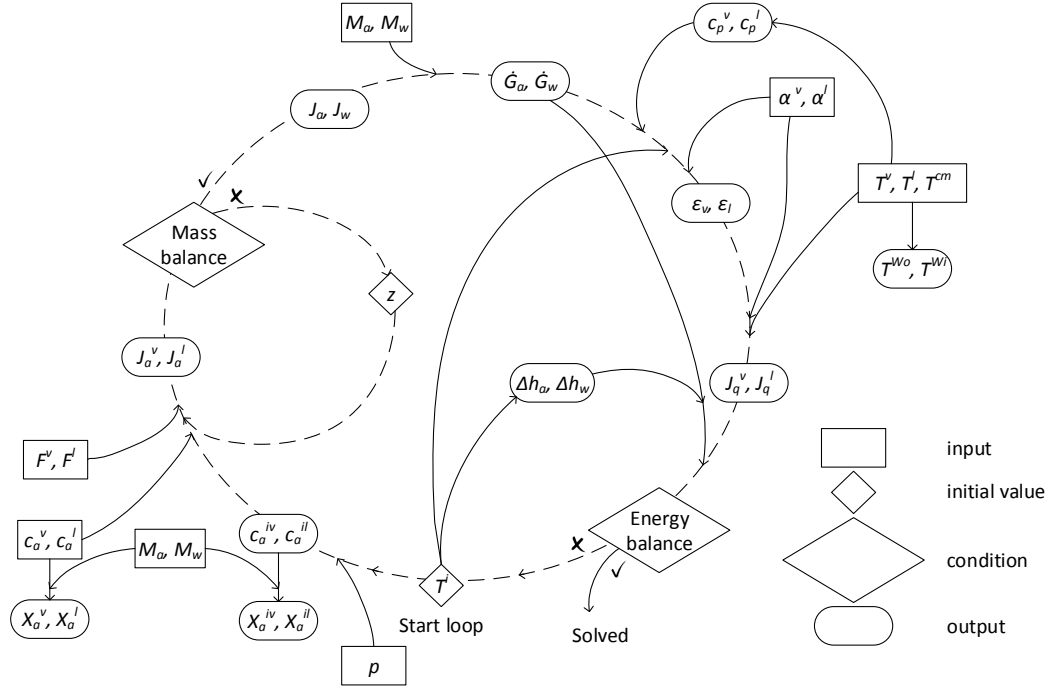


Figure 4.3: Flow diagram of a computational model of a segment of a resorber.

can be converted to a mass concentration with the molar masses (M_a, M_w) of each component. The following equation is used.

$$X_a = \frac{c_a/M_w}{c_a/M_w + (1 - c_a)/M_a} \quad (4.18)$$

The next step is to calculate the molar fluxes from the vapour to the interface and from the interface to the liquid. For this an initial value for z is required as well as the mass transfer coefficients and the concentrations in the vapour and the liquid. According to Fernández-Seara et al. [13] the molar fluxes of ammonia can be determined with:

$$J_a^v = F^v z \ln \left(\frac{z - c^{iv}}{z - c^v} \right) \quad J_a^l = F^l z \ln \left(\frac{z - c^{il}}{z - c^l} \right) \quad (4.19)$$

Here F is the mass transfer coefficient and z is the ratio of ammonia to the total molar flux, $z = J_a/J$. There is no accumulation of mass in the interface so J_a^v and J_a^l should be equal ($J_a^v = J_a^l$). This mass balance condition is indicated in the flow diagram. When the ammonia fluxes to and from the interface are not equal a new z should be taken and the fluxes should be recalculated. This iteration should be repeated until the mass balance is satisfied. The ammonia flux is now determined and with the right z the molar flux of water through the interface can be obtained.

$$J_a = J_a^v = J_a^l \quad J_w = (1 - z)J_a \quad (4.20)$$

By multiplying with the molar masses the molar fluxes can be converted to mass fluxes.

$$\dot{G}_a = J_a M_a \quad \dot{G}_w = J_w M_w \quad (4.21)$$

Now the heat transfer correction factor, ϵ , can be calculated. For this the heat transfer coefficients on the vapour and liquid side of the interface should be known. Also the specific heat capacity of the

mixture is required in the vapour and the liquid phases.

$$\varepsilon^v = \frac{(\dot{G}_a + \dot{G}_w)c_p^v}{\alpha^v} \quad (4.22)$$

Here the vapour heat transfer coefficient and the vapour specific heat capacity should be used for the vapour heat transfer correction factor. And for the correction factor in the liquid, the superscripts should be l instead of v . The heat capacities are affected by the temperature. A fast way to calculate them is using a correlation for each phase with the temperature as variable.

$$c_p^v = \left(0.6464e^{0.003353T^v} + 1.179 \cdot 10^{-15}e^{0.0692T^v}\right) \cdot 1000 \quad (4.23)$$

$$c_p^l = \left(0.0001906T^{l^2} - 0.1333T^l + 28.44\right) \cdot 1000 \quad (4.24)$$

These correlations were constructed using data from Refprop [24] [9].

Now the sensible heat fluxes to and from the interface can be calculated using the following equations [13].

$$J_q'^l = \alpha^l \frac{\varepsilon^l}{1 - e^{-\varepsilon^l}} (T^i - T^l) \quad J_q'^v = \alpha^v \frac{\varepsilon^v}{1 - e^{-\varepsilon^v}} (T^v - T^i) \quad (4.25)$$

These fluxes are not necessarily equal. The temperature at the interface, T^i , is the temperature on the solid vertical line in the interfacial region in figure 4.1c. First the heat that is released due to condensation of both components in the mixture should be determined in order to make an energy balance over the interface. This condensation heat can be determined by multiplying the mass of a component that is condensed by the partial enthalpy of phase change of that component.

$$J_{q_a}^* = \dot{G}_a \Delta h_a \quad J_{q_w}^* = \dot{G}_w \Delta h_w \quad (4.26)$$

The partial enthalpies of phase change of both components are determined from a given interface temperature with the following correlations.

$$\Delta h_a = -0.355T^{i^3} + 418.7T^{i^2} - 1.527 \cdot 10^5 T^i + 1.809 \cdot 10^7 \quad (4.27)$$

$$\Delta h_w = 4.283 \cdot 10^{15} e^{-0.05341T^i} + 3.841 \cdot 10^6 e^{-0.001629T^i} \quad (4.28)$$

To obtain these correlations the partial enthalpies are calculated according to the method used by van Leeuwen [23]. To implement them by using correlations saves a considerable amount of computational time. The gradient of the enthalpy of the mixture with respect to the concentration is used to determine the difference between partial and total enthalpy. Now the energy balance can be made. No energy is accumulated in the interface, so what comes in and what is released must be equal to what goes out.

$$J_q'^l = J_q'^v + J_{q_a}^* + J_{q_w}^* \quad (4.29)$$

When this balance is not satisfied a new interface temperature should be taken and the whole loop should be recalculated. When the energy balance is satisfied the loop is solved.

Additionally the wall temperatures can be calculated with the heat transfer coefficients between the cooling medium side of the wall (α^{cm}), the wall itself (α^W), and the film side of the wall (α^f). The cooling medium side is regarded as the outer wall and may be determined with the following equation.

$$T^{Wo} = \frac{\left(\frac{\alpha^{cm}}{\alpha^W} + \frac{\alpha^{cm}}{\alpha^f}\right) T^{cm} + T^l}{\frac{\alpha^{cm}}{\alpha^W} + \frac{\alpha^{cm}}{\alpha^f} + 1} \quad (4.30)$$

And the film side with equation (4.31).

$$T^{Wi} = \left(\frac{\alpha^{cm}}{\alpha^W} + 1\right) T^{Wo} - \frac{\alpha^{cm}}{\alpha^W} T^{cm} \quad (4.31)$$

These two equations for the wall temperatures are derived from simple heat transfer balances over the wall between the liquid film and the cooling medium.

$$\alpha^{cm}(T^{Wo} - T^{cm}) = \alpha^W(T^{Wi} - T^{Wo}) = \alpha^f(T^l - T^{Wi}) \quad (4.32)$$

4.2.2 Inputs and initial values

In this section the initialisation of the model will be treated. For the considered application the inlet concentration of the vapour is known. And using the fact that it is saturated vapour the temperature can be obtained with a property call.

$$T^v = T(c_a^v, p, q = 1) \quad (4.33)$$

Initially there is no liquid present when the vapour enters the resorber. When the fluid starts to condense the liquid will obtain the concentration that belongs to the same pressure and temperature at saturated liquid conditions. It is expected that when the liquid is brought in contact with the cold wall it will be sub-cooled considerably, because the temperature difference is quite large (± 40 K).

$$c_a^l = c(T^v, p, q = 0) \quad T^l = T^{cm} + 50 \quad (4.34)$$

The initial liquid temperature is a rough guess; fortunately, it does not influence the rest of the process in the heat exchanger much. The cooling medium temperature at the outlet is determined by the application to be 104 °C. The temperatures and concentrations vary along the heat exchanger and a step to the next cell is determined by the mass and energy fluxes in a cell. Equation (4.33) and (4.34) only apply to the first cell of the model.

The plate characteristics are also used in the model. They are shown in table 4.1. The number of plates, N_p , determines the size of the heat exchanger. A manual iteration over the entire model is required to find the right number of plates. Figure 4.4 shows a schematic illustration of a chevron-type plate.

Table 4.1: Input parameters of plate characteristics with some ranges provided by literature.			
Number of plates N_p		Chevron angle β	0-90 ° [16]
Area of plate A_p	0.03-1.5 m ² [37]	Plate wave amplitude a	$d_p/2$
Width of plate W_p	$\sqrt{A_p/3}-\sqrt{A_p/2}$ [37]	Plate wavelength Λ	$2\pi a$ m [16]
Plate spacing δ_p	1.5-5 mm [37]	Thermal conductivity of wall λ_W	15 W/m K [16]
Wall thickness δ_W	0.5-3 mm [37]		

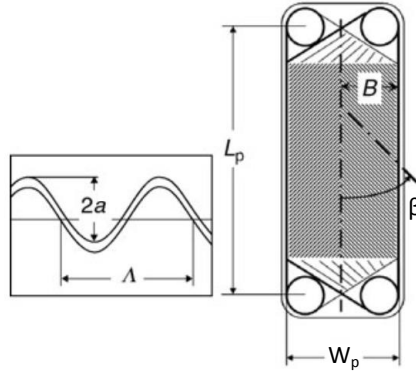


Figure 4.4: Schematic illustration of a plate of a chevron-type plate heat exchanger [16].

Further, the refrigerant mass flow, $\dot{m}_R$, and the pressure inside the resorber, p , are input. They resulted from the calculations of the cycle model from *chapter 3*.

Another input to the model is the number of cells that the heat exchanger is divided into. This may in principle be an arbitrary number, although a too large or too low number does have consequences. A larger number of cells has the benefit of producing detailed results, however the computational time is longer. A lower number of cells causes the computational speed to be fast, only the level of detail of the results is lower, because there are less data points. The number of cells is chosen such that both the computational time of the calculation and the level of detail of the results are satisfactory. The number

of cells that is used in the calculation example of this chapter is $n_c = 150$. The computational time for the calculation is 52 seconds when the model is run on a computer with an Intel® Core™ i5-4690 processor. And the level of detail can be judged by the smoothness of the results in figures 4.7-4.13.

It is wise to adjust the initial values for the iterations for each cell to reduce computational time. The interface temperature is expected always to be below the saturation temperature of the liquid at the same concentration. This is the case for a concentration profile across the interface typical to a condenser according to Sieres and Fernández-Seara [36]. Furthermore, the interface temperature is expected not to drop below the liquid temperature T^l , because the liquid is on the cold side of the interface. So the initial value of the interface temperature can be taken as:

$$T^i = (T^{l*} + T^l)/2 \quad (4.35)$$

In the same case a solution for z exists in the interval $c_a^{il} < z < c_a^v$ [36]. So a good initial value for the ammonia to total flux ratio can be estimated as:

$$z = (c_a^{il} + c_a^v)/2 \quad (4.36)$$

A plot of the typical concentration profile in a resorber is shown in figure 4.5.

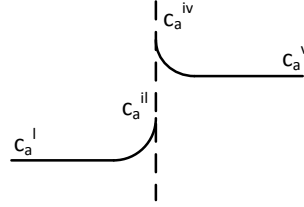


Figure 4.5: A concentration profile across the vapour-liquid interface typical for a condenser (resorber) [36].

4.2.3 The next cell

Concentrations and temperatures will change in the next cell. The concentration difference can be determined by the molar fluxes through the interface. The molar ammonia concentrations are defined by the molar flow of ammonia divided by the total flow.

$$c_a = \frac{\dot{n}_a}{\dot{n}} \quad (4.37)$$

In both phases the ammonia flow rate changes as well as the total flow rate. In the resorber the process of condensation of the mixture takes place, so the total flow in the vapour phase will decrease and the flow in the liquid phase will increase. The degree of change after one cell for these rates is equal and can be described by:

$$\Delta \dot{n}^v = \Delta \dot{n}^l = (J_a + J_w)A_c \quad (4.38)$$

The ammonia molar flow changes in both phases because of the flux of ammonia through the interface. The degree of change after one cell is simply:

$$\Delta \dot{n}_a^v = \Delta \dot{n}_a^l = J_a A_c \quad (4.39)$$

These differences must be subtracted from the molar flows in the vapour and added to the molar flows in the liquid. With the new molar flows in both phases the molar concentration can be calculated with equation (4.37). The molar concentration can be converted to a mass concentration using equation (4.18). To calculate these changes of flow the cell area A_c is required. Four different methods are considered to determine the area of each cell. The method should be used for which the model is most stable.

$$Constant : A_c = A_p/n_c \quad (4.40)$$

$$\text{Linear increase : } A_c = A_p/(100n_c) + \frac{A_p/n_c - A_p/(100n_c)}{(n_c + 1)/2} \cdot i \quad (4.41)$$

$$\text{Sine : } A_c = A_p/n_c \cdot \sin(\pi/n_c \cdot i - \pi/2) + A_p/n_c \quad (4.42)$$

$$\text{Pyramid : } A_c = \begin{cases} A_p/(10n_c) + 0.9 \frac{A_p/n_c}{(n_c+1)/4-1} \cdot (i-1), & \text{for } i = 1 : \frac{n_c+1}{2} \\ A_p/(10n_c) + 0.9 \frac{A_p/n_c}{(n_c+1)/4-1} \cdot (\frac{n_c+1}{2} - 1) - 0.9 \frac{A_p/n_c}{(n_c+1)/4-1} \cdot (i - \frac{n_c+1}{2}), & \text{for } i = \frac{n_c+1}{2} : n_c \end{cases} \quad (4.43)$$

In these equations A_p is the area of one plate and n_c is the number of cells that the heat exchanger

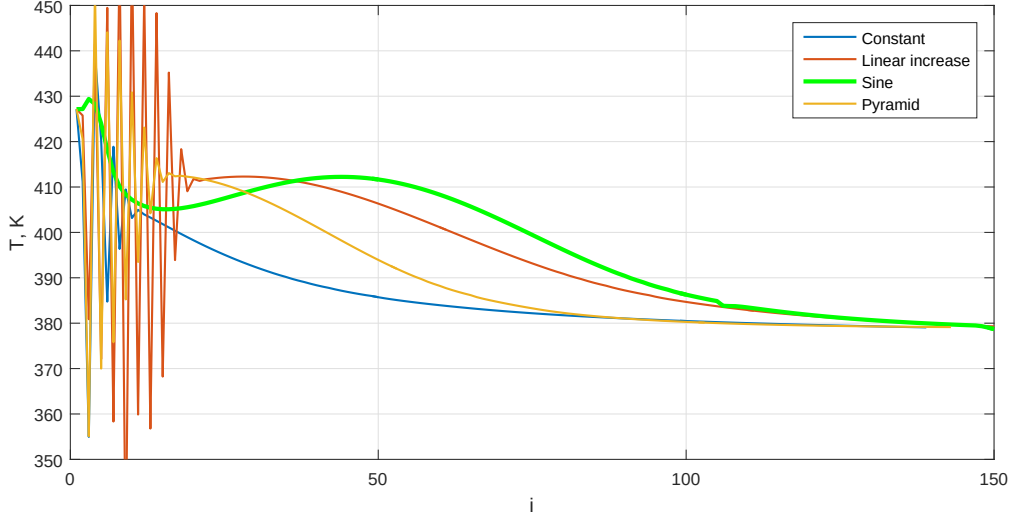


Figure 4.6: Liquid temperature plotted per cell to compare the methods for variation of A_c .

is divided into. The current cell is represented by the counter i . The average value of these different cell area methods over the whole heat exchanger is always equal to A_p/n_c . Figure 4.6 shows one of the variables in the model (the liquid temperature of the working fluid, T^l) in four cases when each of the proposed methods for the cell area are used. From this figure it is clear that the sine method is most stable under the considered operating conditions.

Temperature changes as a result of the change of energy flows. The temperatures can be determined with a property call using the new concentration and enthalpy (equation (4.48)). The change of energy flow is not equal for both phases. For the vapour phase it is equal to the energy flow from the vapour to the interface together with the contribution of the mass that has condensed.

$$\Delta \dot{m}^v h^v = (J_q^v + J_{q_a}^* + J_{q_w}^*) A_c \quad (4.44)$$

And this energy flows out of the vapour, so it must be subtracted from the energy flow in the vapour. When the mass flow is known the enthalpy can be evaluated. The mass flow changes just as the molar flow does. The change in mass flow is:

$$\Delta \dot{m}^v = \Delta \dot{m}^l = (\dot{G}_a + \dot{G}_w) A_c \quad (4.45)$$

In the vapour it must be subtracted from the original vapour mass flow to obtain the new vapour mass flow and to the liquid it should be added. The change of energy flow in the liquid is determined by what comes in from the interface and what goes out to the cooling medium.

$$\Delta \dot{m}^l h^l = (J_q^l + J_{q_a}^* + J_{q_w}^* - J_q^{cm}) A_c \quad (4.46)$$

The heat that is transferred from the cooling medium through the wall to the liquid film can be calculated by:

$$J_q^{cm} = \frac{T^l - T^{cm}}{1/\alpha^{cm} + 1/\alpha^W + 1/\alpha^f} \quad (4.47)$$

The new mass flow of the liquid can be calculated with equation (4.45). After that the new enthalpy of the liquid can be obtained. When the concentrations and enthalpies of both phases are determined, the new temperatures can be evaluated using a property call.

$$T = T(c_a, p, h) \quad (4.48)$$

It may occur that the vapour enthalpy of the next cell is lower than the saturation enthalpy at the new concentration. This implies that the vapour has become a two-phase substance. When this happens the part on the vapour side of the interface that is liquid is added to the film. This small liquid substance has the liquid saturation conditions (concentration and enthalpy) at the vapour temperature. The new liquid film conditions are slightly changed using a mass and an energy balance. The conditions on the vapour side of the interface have become saturated vapour conditions at the vapour temperature. This so called supplemental condensation has an effect on the calculation of entropy production in the interface (see equation (4.8)), because the molar fluxes through the interface (J_a , J_w) have increased. The molar flux that results from supplemental condensation is separated into an ammonia and a water part with the liquid saturation concentration and added to the ordinary molar fluxes through the interface. The ordinary molar fluxes through the interface were determined with equation (4.20). In practice this procedure appears to have a modest impact (± 15 %) on the entropy production rate in the interface.

4.2.4 Transfer coefficients and pressure drop

The model uses five heat transfer coefficients (α^{cm} , α^W , α^f , α^l , α^v) and two mass transfer coefficients (F^l , F^v). These transfer coefficients vary along the plate length of the heat exchanger. In this section the calculation of each of them is explained.

The cooling medium of the application is evaporating water and heat transfer is dominated by convection. The heat transfer coefficient of the cooling medium is obtained with a recent prediction method that was introduced by Amalfi et al. [3]. The method is valid for flow boiling in plate heat exchangers. The following correlation for the Nusselt number is used when the Bond number Bd is greater than 4. For the considered application $Bd = 5.86$.

$$Amalfi : Nu = 18.495 \beta_r^{0.248} Re^{cm,v^{0.135}} Re^{cm,lo^{0.351}} Bd^{0.235} Bo^{0.198} \rho_r^{-0.223} \quad (4.49)$$

The dimensionless factors for this correlation can be obtained with:

$$\text{Reduced chevron angle : } \beta_r = \beta / \beta_{max} \quad (4.50)$$

$$\text{Reynolds number of vapour : } Re^{cm,v} = \dot{G}^{cm} q^{cm} d_h / \mu^{cm,v} \quad (4.51)$$

$$\text{Reynolds number of liquid only : } Re^{cm,lo} = \dot{G}^{cm} d_h / \mu^{cm,l} \quad (4.52)$$

$$\text{Bond number : } Bd = (\rho^{cm,l} - \rho^{cm,v}) g d_h^2 / \gamma \quad (4.53)$$

$$\text{Boiling number : } Bo = \frac{J_q^{cm}}{\dot{G}^{cm} \Delta h^{cm}} \quad (4.54)$$

$$\text{Density ratio : } \rho_r = \rho^{cm,l} / \rho^{cm,v} \quad (4.55)$$

The maximum chevron angle β_{max} is 70 degrees. The liquid and vapour properties of water ($\mu^{cm,v}$, $\mu^{cm,l}$, $\rho^{cm,v}$, $\rho^{cm,l}$, σ) and the enthalpy of phase change, Δh^{cm} , at the cooling medium temperature T^{cm} are obtained with Refprop [24] [9]. The mass flux of water $\dot{G}^{cm}$ is calculated with the mass flow per channel and the cross sectional area between two plates. The heat flux to the cooling medium J_q^{cm} is calculated with equation (4.47). And the hydraulic diameter can be determined with the plate characteristics (see table 4.1) [16].

$$d_h = 4a / \Phi \quad \Phi = \frac{1}{6} \left(1 + \sqrt{1 + X^2} + 4\sqrt{1 + X^2/2} \right) \quad X = 2\pi a / \Lambda \quad (4.56)$$

In the wall the heat transfer takes place only by conduction. The conductivity of the plate material and the thickness of the plate are used to determine the heat transfer coefficient. This is the only heat transfer coefficient that is constant along the length of the plate.

$$\alpha^W = \lambda_W / \delta_W \quad (4.57)$$

Also in the liquid film the heat transfer is assumed to be only governed by conduction. It is calculated similarly to the heat transfer coefficient of the wall. However, this transfer coefficient is variable because both the conductivity of the liquid mixture and the film thickness are variable.

$$\alpha^f = \lambda^l / \delta_f \quad (4.58)$$

According to Mills [25] in laminar film condensation the film grows like $y^{1/4}$, where y is the length coordinate in the flow direction along the length of the plate. So it is suggested to express the film thickness as:

$$\delta_f = \frac{\delta_p}{2} \cdot \frac{y^{1/4}}{L_p^{1/4}} \quad (4.59)$$

The heat transfer coefficient on the liquid side of the vapour-liquid interface, α^l , can be taken to be equal to α^f as was done by Fernández-Seara et al. [14]. Alternatively, it may be calculated with the correlation of Seader and Henley [35] which is made for flow across a flat plate of length y . The Nusselt number can be calculated with:

$$\text{Seader and Henley : } Nu = 0.037 Re^{0.8} Pr^{1/3} \quad (4.60)$$

The Reynolds number that is used for this correlation does not have the hydraulic diameter as length parameter, but the length of the plate.

$$Re = \frac{v^l y}{\nu^l} \quad (4.61)$$

On the other side of the interface the heat transfer coefficient, α^v , could be calculated with the correlation of Seader and Henley [35] as well. Also the correlation of Whitaker [41] is an option, which is made for turbulent flow past a flat plate. It is recommended for turbulent flow along a flat plate by Mills [25]. In this case the liquid film is regarded as a plate with respect to the vapour flowing over it. The correlation for the Nusselt number is:

$$\text{Whitaker : } Nu = 0.029 Re^{0.8} Pr^{0.43} \quad (4.62)$$

The definition of the Reynolds number of equation (4.61) is used for this correlation with vapour conditions instead of liquid.

The mass transfer coefficients are obtained using the Chilton and Colburn analogy [8]. This analogy can be represented by the next equation.

$$\text{Chilton and Colburn : } F^l = \frac{\alpha^l D^l \rho_{mol}^l}{\lambda^l} \left(\frac{Sc^l}{Pr^l} \right)^{1/3} \quad (4.63)$$

The analogy is the same for the vapour as for the liquid, so for the vapour side all superscripts l may be replaced by v .

Pressure drop

In this section attention will be paid to the pressure drop in the heat exchanger. Three different methods are used to determine the pressure drop along the length of a plate. The first method is taking the average value between the vapour and liquid single phase calculations in a plate heat exchanger. The vapour phase pressure drop in a plate heat exchanger can be obtained with the following correlation of Sinnott and Towler [37]:

$$\text{Sinnott and Towler : } \Delta p = 8 j^v (\Delta y / d_h) \frac{\rho^v v^2}{2} \quad (4.64)$$

with $j^v = 0.6Re^{v-0.3}$. The same correlation may be used for the liquid and then the superscripts v should be replaced by l . The Reynolds number here is defined as in equation (4.67). In the VDI heat atlas [16] it is suggested that linear interpolation between the two single phase pressure drops might be a reasonable approximation based on the experiments of Kreissig and Müller-Steinhagen [22] in plate heat exchangers.

The second method that is applied is the correlation of Yan et al. [42]. They performed experiments of condensation of a single fluid in a plate heat exchanger.

$$Yan et al. : \Delta p = 2j^{tp}(\Delta y/d_h) \frac{\dot{G}^2}{(\rho^l + \rho^v)/2} \quad (4.65)$$

$$j^{tp} = 94.75 Re_{eq}^{-0.0467} Re^{-0.4} Bo^{0.5} \frac{p}{p_{cr}}^{0.8} \quad (4.66)$$

$$Re = \frac{\dot{G}d_h}{\mu^l} \quad Re_{eq} = \frac{\dot{G}_{eq}d_h}{\mu^l} \quad Bo = \frac{J_q^{cm}}{\dot{G}\Delta h_T^*} \quad (4.67)$$

$$\dot{G}_{eq} = \dot{G} \left[1 - q_{wf} + q_{wf} \left(\frac{\rho^l}{\rho^v} \right)^{0.5} \right] \quad \dot{G} = \frac{\dot{m}_R}{W_p \delta_p N_p} \quad (4.68)$$

The critical pressure of ammonia-water was calculated using the method of Conde [11]. And the phase change enthalpy at constant temperature, Δh_T^* , was determined using a property call of Rattner and Garimella [32].

The third method is taken from the publication of Müller-Steinhagen and Heck [28]. This is a two-phase pressure drop calculation method for in tubes. However, it was also used to compare with experiments in plate heat exchangers by Kreissig and Müller-Steinhagen [22]. That comparison showed that it generally overestimated the pressure drop in a plate heat exchanger.

4.3 Example

The calculation is applied to the application that was introduced in *chapter 1*. A molar concentration of 0.7 is used for the working fluid as was identified in *chapter 3* to offer the highest cycle performance. Table 4.2 gives an overview of the inputs that are used in this example.

Table 4.2: Input that is used for the example

Plate characteristics				Initial points		Other	
N_p	4250	β	50 °	c_a^v	0.70 mol/mol	p	43.8 bar
A_p	1.3 m ²	a	2 mm	c_a^l	0.26 mol/mol	$\dot{m}_R$	10.7 kg/s
W_p	1.75 m	Λ	12.6 mm	T^v	477.6 K	$\dot{m}_H$	7.6 kg/s
δ_p	4 mm	λ_W	15 W/m K	T^l	427.2 K	M_a	17 g/mol
δ_W	1 mm			T^{cm}	377.2 K	M_w	18 g/mol

Table 4.3: Methods for transfer coefficients

Coefficient	Method
α^{cm}	Amalfi et al. [3], eq. (4.49)
α^W	Conduction, eq. (4.57)
α^f	Conduction, eq. (4.58)
α^l	Seader and Henley [35], eq. (4.60)
α^v	Seader and Henley [35], eq. (4.60)
F^l	Chilton and Colburn [8], eq. (4.63)
F^v	Chilton and Colburn [8], eq. (4.63)

The number of plates are chosen such that the process of condensation of the working fluid inside the heat exchanger is completed. Other plate characteristics are estimated within the typical ranges

(see table 4.1). The initial temperatures and concentrations are determined using equation (4.33) and (4.34). Other inputs shown in table 4.2 are a result of the application ($\dot{m}_H$, M_a , M_w) and the cycle performance calculations (p , $\dot{m}_R$). Table 4.3 shows which methods are used for the different heat and mass transfer coefficients.

First the process is depicted in a temperature-concentration diagram in figure 4.7. The vapour follows the saturation line starting at the initial concentration of 0.7 and ending with an ammonia concentration near 1. The liquid is subcooled by the cold wall. It approaches saturation at the end and reaches the concentration of 0.7 at total condensation.

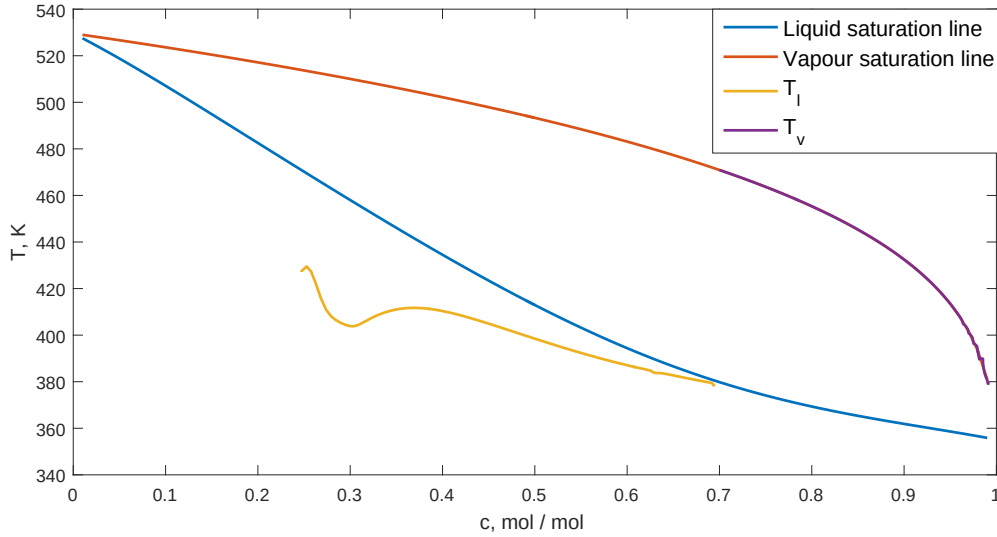


Figure 4.7: Temperature - concentration diagram of the process inside the heat exchanger.

Figure 4.8 shows the process in a temperature-quality diagram. This figure can be compared with figure 3.6. The vapour temperature corresponds to the trend of the working fluid temperature in figure 3.6. This is explained by the fact that the temperature of the working fluid in figure 3.6 is at saturated conditions. The vapour temperature also follows the saturation line, as is clear from figure 4.7. The trend of the liquid temperature is different because it is sub-cooled.

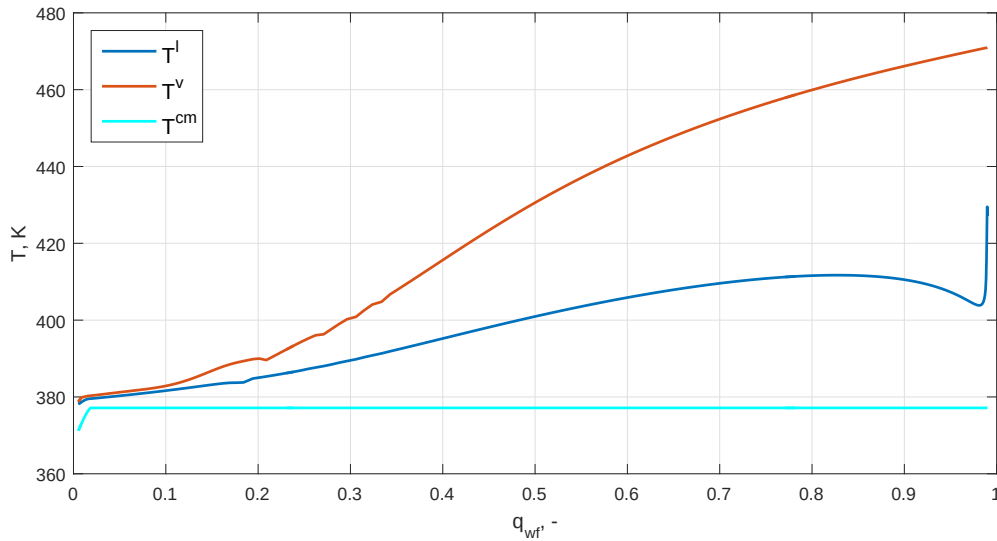


Figure 4.8: Temperature - quality diagram of the process inside the heat exchanger.

Figures 4.9 and 4.10 show the temperature and concentration profiles along the length of a plate. The temperatures and concentrations constitute the forces for heat and mass transfer in the heat exchanger. It can be observed that the temperature and concentration gradients are much higher in the first half of the heat exchanger than in the second half. The temperature profiles are shown in figure 4.9 of the liquid, vapour, interface, inner wall, outer wall and cooling medium. The cooling medium starts at the outlet of the heat exchanger with a temperature of 90 °C as dictated by the application. When the cooling medium reaches 104 °C it starts to evaporate at constant temperature. About half way through the heat exchanger when the length is about 1 m the vapour temperature drops below the interface temperature. The vapour temperature stays above the liquid temperature however.

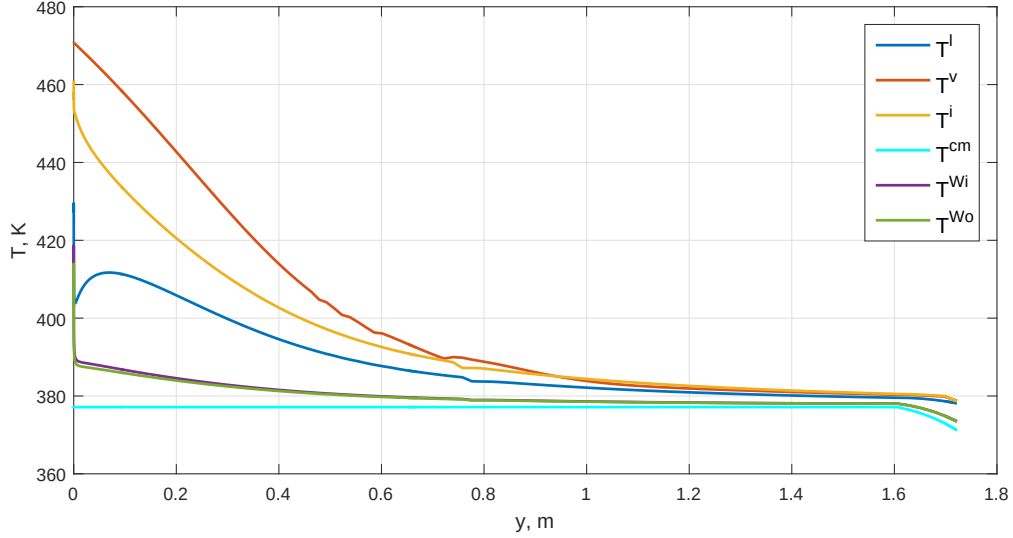


Figure 4.9: Temperature profiles along the plate length.

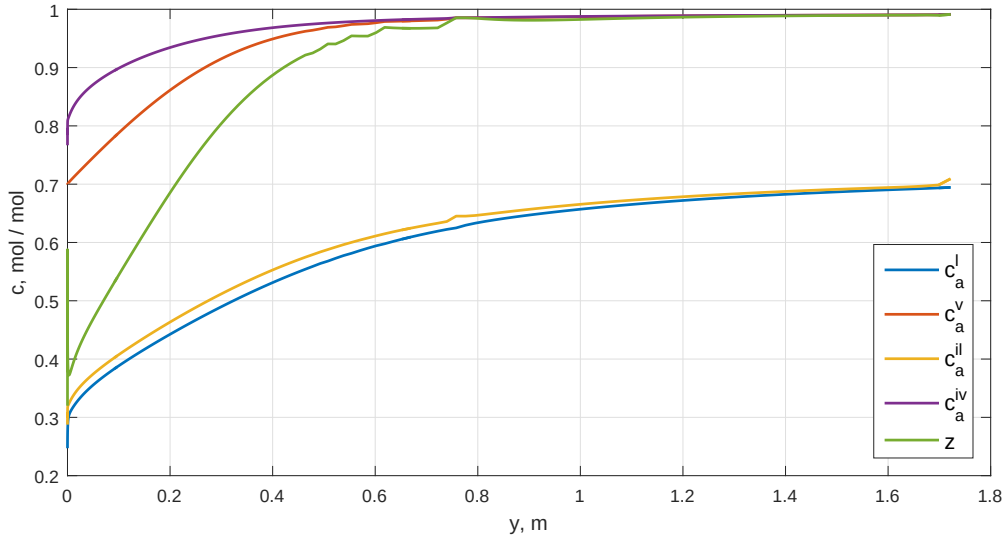


Figure 4.10: Concentration profiles and flux ratio z along the plate length.

In figure 4.10 the concentrations are presented of the liquid, vapour, liquid interface and vapour interface. Also the ammonia flux ratio z is shown in figure 4.10. The flux ratio starts with a value of approximately 0.4 and increases towards 1. This means that in the beginning there is approximately

the same molar amount of water being condensed as ammonia, and at the end hardly any water is still being condensed, but only ammonia.

Figure 4.11 displays the mass flows of the liquid and vapour of the working fluid and of the cooling medium. This figure gives insight into the progress of the condensation process in the heat exchanger. It can be observed that most of the mass of the working fluid has already condensed half way through the heat exchanger.

In figure 4.12 the heat fluxes are shown of the sensible heat from the vapour to the interface, the sensible heat from the interface to the liquid, the latent heat of ammonia through the interface, the latent heat of water through the interface and the heat flux from the liquid film to the cooling medium. The fluxes are also shown in the schematic illustration of figure 4.1b. Figure 4.12 shows that the heat

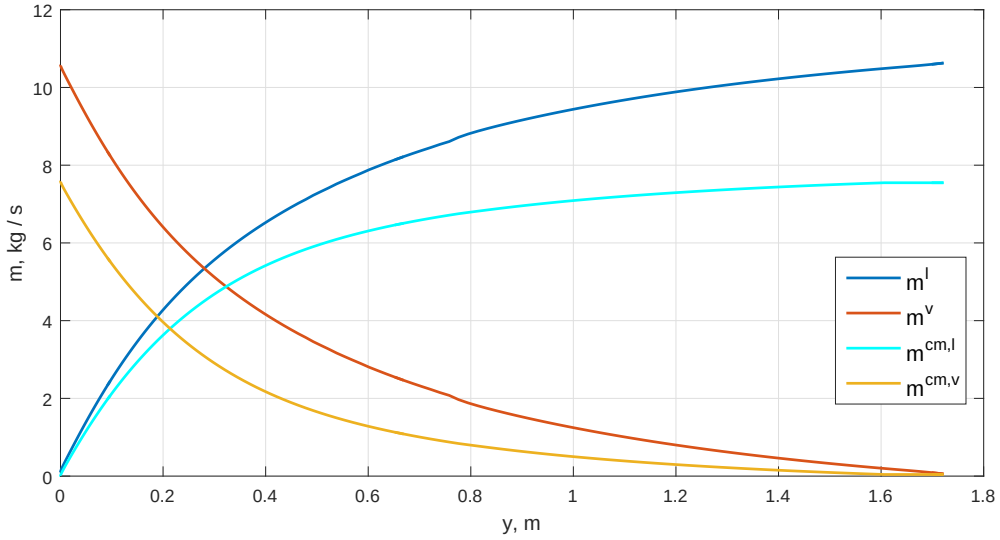


Figure 4.11: Mass flows of different phases on both sides of the wall along the plate length.

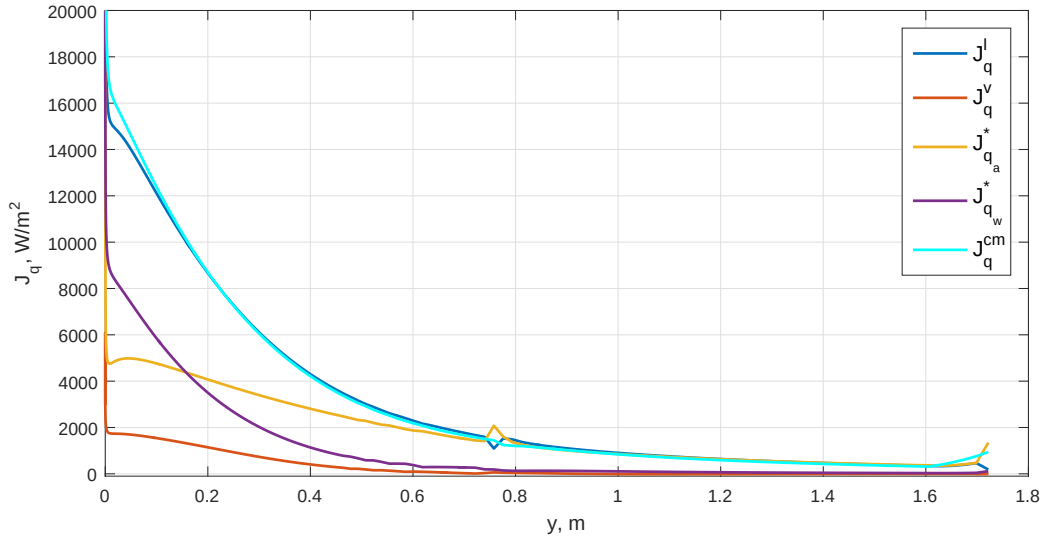


Figure 4.12: Heat fluxes along the plate length.

flux from the interface to the liquid, J_q^l , and the heat flux from the liquid to the cooling medium, J_q^{cm} , are approximately equal. This means that both latent heat fluxes ($J_{q_a}^*$, $J_{q_w}^*$) play a dominant role in

the determination of change in enthalpy in the liquid (see equation (4.46)). J_q^v , $J_{q_a}^*$ and $J_{q_w}^*$ determine the change of enthalpy in the vapour phase (equation (4.44)).

Figure 4.13 illustrates the local entropy production that is calculated with the theory of non-equilibrium thermodynamics. The irreversible phenomenon of heat transfer is present dominantly in the first part of the process, this explains the high entropy production rates there. Only the entropy production rate in the interface contains terms of mass transfer. Therefore, the trend of the entropy production in the interface is somewhat different from the others. The entropy production in the vapour phase is zero, because there are no temperature gradients in the vapour phase. The entropy production rate in the wall is relatively small, but it has the same trend as the entropy production rates in the liquid.

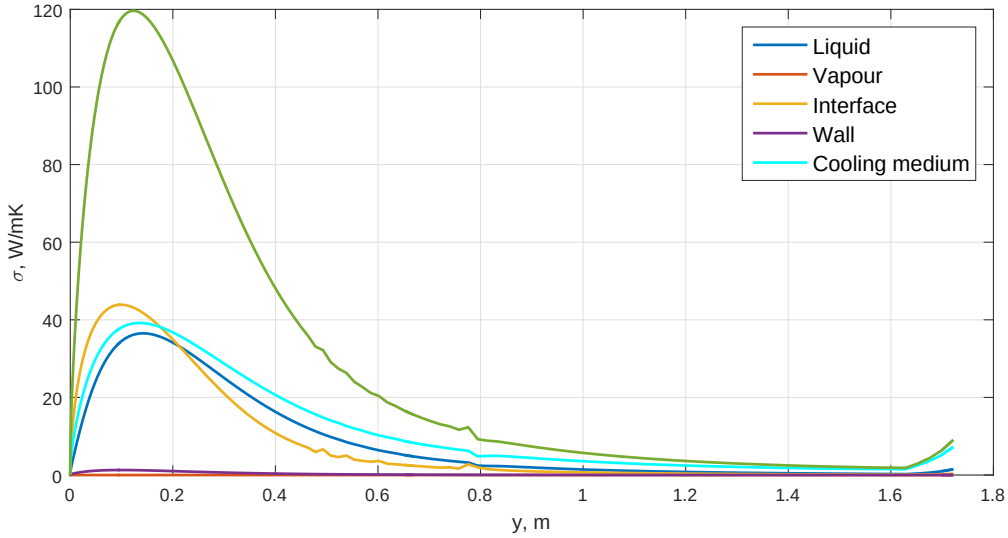


Figure 4.13: Local entropy production along the plate length.

When the total entropy production rate is added up it amounts to 6.40 kW/K. This value is a 21 % higher than what was calculated with the cycle model (5.29 kW/K, table 3.2). This means that one or more of the contributions give an overestimation of entropy production. The largest error is expected to arise from the calculation method for the cooling medium. This calculation method definitely has the weakest theoretical basis among the considered contributions. However, as the order of magnitude is correct, it is expected that the insights that figure 4.13 gives into the distribution of entropy production in the heat exchanger are valid. The boundary layer thickness in the method for calculation of entropy production in the cooling medium was a rough guess. Figure 4.14 shows how the entropy production in the cooling medium is affected by the assumption for the liquid boundary layer thickness. Without taking the cooling medium into account the total entropy production amounts to 4.08 kW/K. Pressure drop in both fluids is also an irreversible phenomenon that produces entropy. The contribution is not taken into account in the calculation of entropy production in either model, because it is expected to be relatively small. The pressure drop itself is calculated though with three different methods. The results are shown in figure 4.15. This figure shows that the pressure drop is extremely small. This is due to the fact that the mass flux through the plates is very small ($\dot{G} = 1.68 \text{ kg/sm}^2$), compared with the experiments in literature [22] [42] ($\dot{G} \approx 100 \text{ kg/sm}^2$).

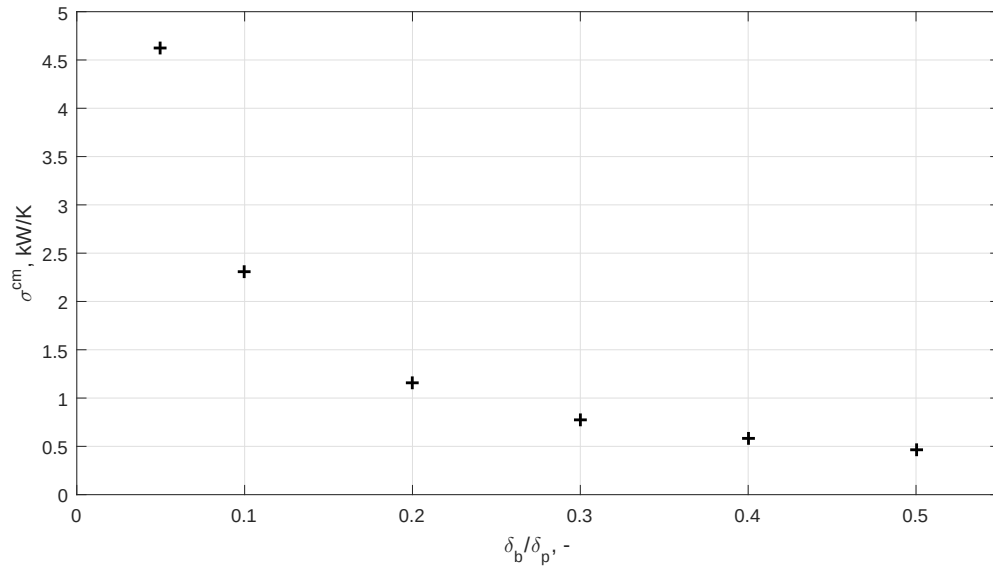


Figure 4.14: Entropy production in the cooling medium at different liquid boundary layer thicknesses.

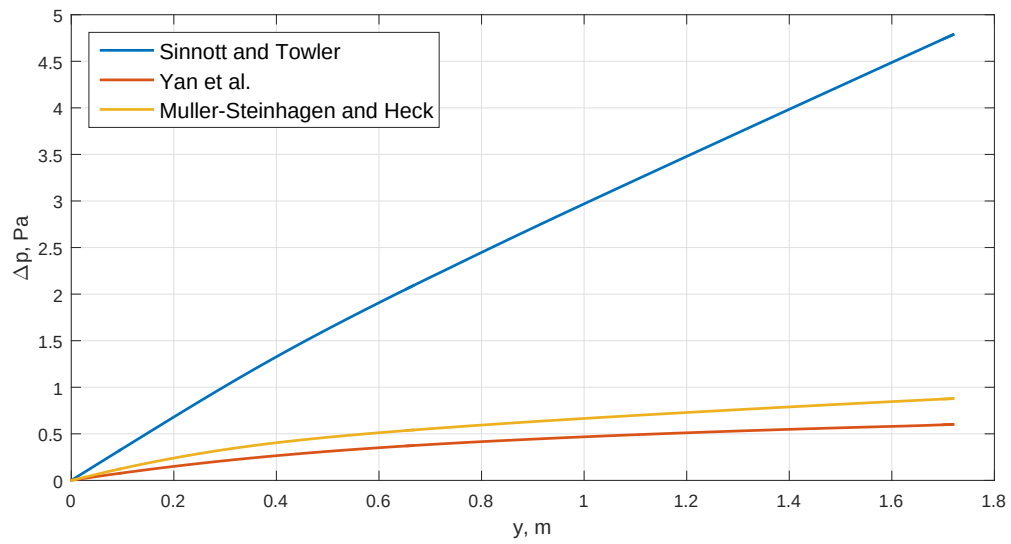


Figure 4.15: Pressure drop along the plate length calculated with different methods.

Chapter 5

Results and discussion

In this chapter an economical study is performed where the investment costs and energy costs at different operation conditions are compared. Also the payback time of the installation is estimated to show the relevance of a CRHP for the considered application. Afterwards concepts for reduction of the resorber area will be analysed. At the end the weaknesses of the models of *chapters 3* and *4* are treated.

5.1 Economic cycle optimisation

In this section the economical aspects of the CRHP in the considered application are analysed. The cycle should be optimised to have the best energetic performance under the constraint of a payback time of 3 years. To find the optimal combination of COP and heat exchanger area both models that were developed will be used together. The cycle model of *chapter 3* is used to obtain the COP of the system and the resorber model of *chapter 4* to obtain the area of the resorber. Then the COP is related to the energy cost of the system. And the area of the resorber is related to investment cost of the system. The minimum temperature difference in the resorber, ΔT_{min} , is varied to alter the operating conditions of the system. The total entropy production rate in the system will increase when the ΔT_{min} is increased, because the forces are then larger. The effect is opposite for the COP ; this is shown in figure 5.1.

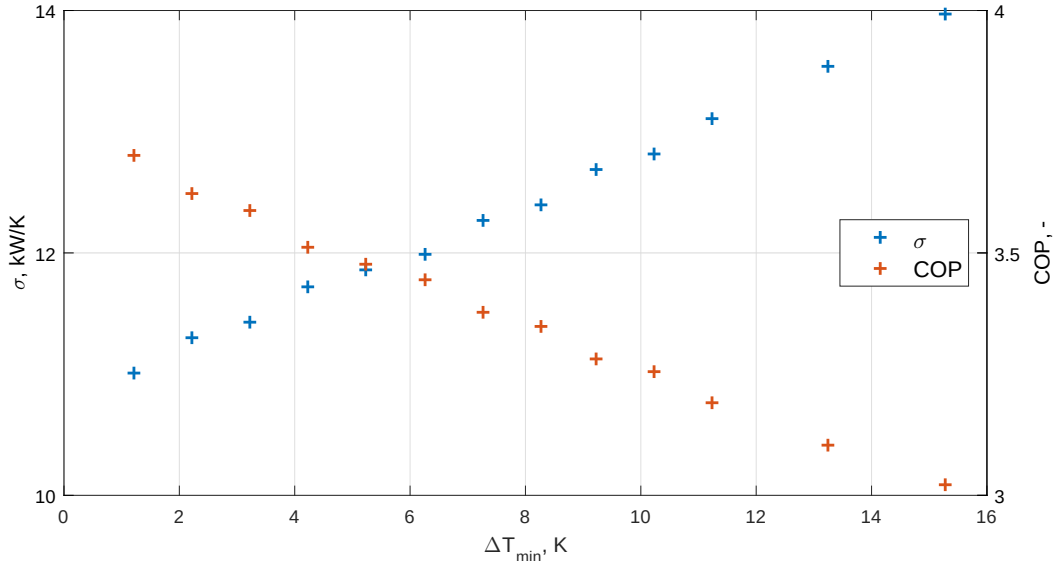


Figure 5.1: Total entropy production in the cycle when the minimum temperature difference in the resorber is varied.

Investment cost estimation

The investment cost of the system is estimated with a cost correlation of Sinnott and Towler [37]. The equation has the following form:

$$C_i = a + bS^n \quad (5.1)$$

Where S is the size parameter. a and b are cost constants and n is an exponent for a certain type of equipment. Only the costs of the resorber, desorber and compressor are taken into account. Other costs, such as for the valve, piping and fluid are neglected. For the resorber and desorber the constants of a plate and frame heat exchanger are used. The compressor is assumed to be centrifugal, because cost data are provided by Sinnott and Towler [37]. Zaytsev [43] suggested that a twin screw compressor would be the best option for wet compression. It is assumed that the cost of a screw compressor is comparable to that of a centrifugal compressor of the same capacity. Table 5.1 shows the constants that are provided by Sinnott and Towler [37].

Table 5.1: Purchased equipment cost for common plant equipment [37].

Equipment	Units for size, S	S_{lower}	S_{upper}	a	b	n
Plate and frame heat exchanger	area, m ²	1.0	500	1350	180	0.95
Centrifugal compressor	driver power, kW	75	30000	490000	16800	0.6

The data is based on US dollars of 2007. To convert the cost to a present value of Euro a factor for inflation and currency conversion is used. The inflation factor is taken from an inflation calculator of the United States Bureau of Labour Statistics [29]. The currency conversion factor is obtained from data provided by the European Central Bank [4].

$$f_{inf} = 1.16 \quad f_{cur} = 0.91 \quad (5.2)$$

In all circumstances not more than one centrifugal compressor is necessary for the considered application. The required drive power as size parameter is obtained with the cycle model from *chapter 3*. The heat transfer rates of the application are large, therefore more than one heat exchanger is often required. When this is the case it is assumed that a maximum number of the heat exchangers with the maximum size parameter of 500 m² is used, together with a small supplementary heat exchanger to fulfil the total required heat transfer area. In figure 2.3 it was shown that a few large heat exchangers are always cheaper than many small ones. The required area for the resorber is calculated with the resorber model of *chapter 4*. The area of the desorber is obtained with a rough estimation.

$$A_{des} = \frac{\dot{Q}_C}{U\Delta T_m} \quad (5.3)$$

Where $U = 1500 \text{ W/m}^2\text{K}$ is the estimated overall heat transfer coefficient [34]. ΔT_m is the estimated mean temperature difference between the refrigerant and the solvent fluid of the application. This temperature difference is estimated making use of figure 3.6 to be 15 K. Q_C depends on the COP of the system and it can thus be determined by:

$$\dot{Q}_C = \dot{Q}_H \left(1 - \frac{1}{COP} \right) \quad (5.4)$$

$\dot{Q}_H$ is determined by the application and the COP can be calculated with the cycle model of *chapter 3*.

Then a factor for the installation cost is taken into account. It is $f_{inst} = 1.8$; this implies that the installation costs are estimated to be 80 % of the total equipment cost. This factor is multiplied with the total equipment cost to obtain the total cost. It is based on factors provided by Sinnott and Towler [37] and accounts for equipment erection (30 %) and piping (50 %). This is assuming that buildings, instrumentation and some piping can be used from the currently installed system.

Figure 5.2 depicts the investment costs of the different components, the installation costs and the total investment costs for different coefficients of performance of the cycle.

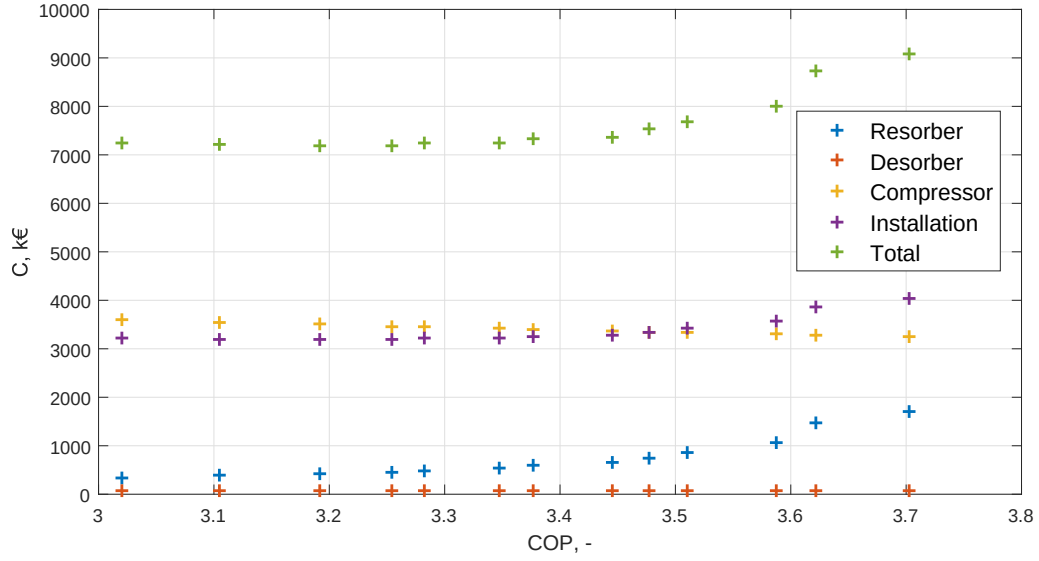


Figure 5.2: Cost of investment

Energy cost estimation

The energy cost of operation of the heat pump is considered over lifetime of the system. The lifetime of the system is expected to be $\tau_{life} = 15$ years. The power demand of the compressor, $\dot{W}_c$, is converted to an electricity demand by the efficiency of the electric drive, which is assumed to be $\eta_{el} = 0.98$. The electricity demand of the compressor is converted to an energy consumption during the whole lifetime of the system assuming that the system operates 8000 hours per year [6]. The cost of electricity in industry in the Netherlands in 2016 is $c_e = 0.0652$ €/kWh according to the European Commission [10]. The information above can be summarized in the following equation.

$$C_{el} = \frac{\dot{W}_c \cdot 10^{-3} \cdot 8000}{\eta_{el}} \tau_{life} c_{el} \quad (5.5)$$

The factor of 10^{-3} is for unit conversion from W to kW. The compressor power can be obtained with the COP of the system and the resorber duty.

$$\dot{W}_c = \frac{\dot{Q}_H}{COP} \quad (5.6)$$

In figure 5.3 the energy costs are shown together with the total investment costs at different operating conditions.

From figure 5.3 it is clear that the energy costs over the whole lifetime of the system are an order of magnitude higher than the investment cost. Not all components were considered in the estimation of the investment, but it is not expected that that would change the situation significantly. The cheapest operation of the CRHP, among the investigated options, is when the COP is 3.7. This corresponds to a ΔT_{min} of 1.21 K. The total cost of the system is then 46.8 M€.

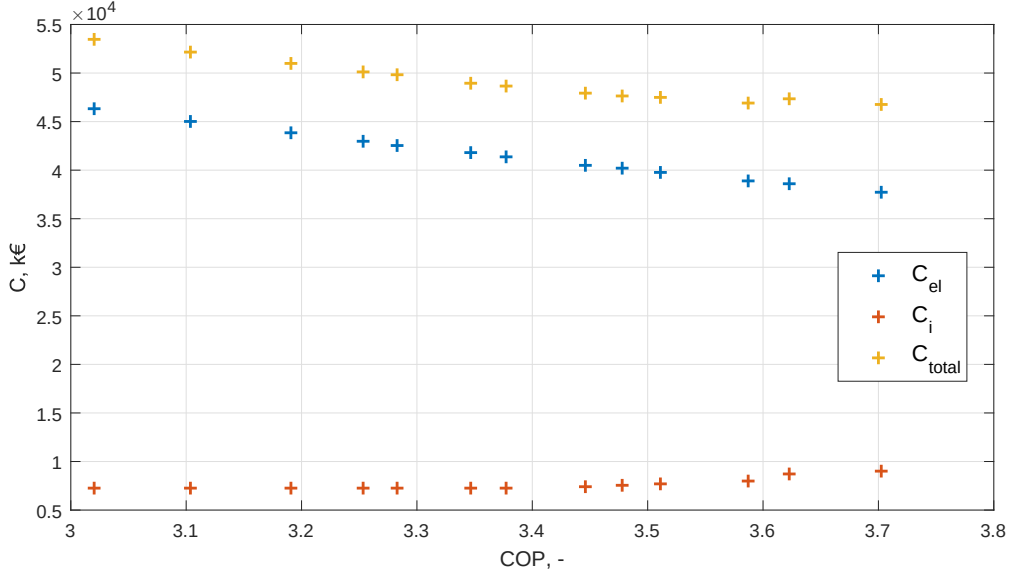


Figure 5.3: Cost of electricity and investment

Payback period

To determine the payback time the profit of the system that is installed should be defined. The economical profit of the new system will be defined by the saving of energy cost with respect to the current system with unconstrained source mass flow. The current VCHP system with unconstrained source mass flow has a COP of 2.76. The yearly energy cost can be calculated with equation (5.5), only with $\dot{W}_c = 6.34$ MW and $\tau = 1$ year. The result is $C_{elVCHP}^{p.a.} = 3307$ k€. The yearly energy cost of the CRHP can be calculated with:

$$C_{elCRHP}^{p.a.} = C_{el}/\tau_{life} \quad (5.7)$$

Where τ_{life} is the lifetime of the system which is taken to be 15 years. The payback period in years is the investment cost of the system divided by the yearly profit.

$$\tau_{pb} = \frac{C_i^{total}}{C_{elVCHP}^{p.a.} - C_{elCRHP}^{p.a.}} \quad (5.8)$$

The payback time is depicted in figure 5.4 for different COP 's of the system.

Figure 5.4 shows that a payback time of 3 years is not attainable, the shortest payback time that can be achieved is 10.28 years. This corresponds to a minimum temperature difference in the resorber of 3.22 K. From figure 5.2 it can be read that the investment cost is then 8.0 M€ and figure 5.3 shows that the energy cost over the lifetime is 38.9 M€. The shortest payback time is still shorter than the lifetime of the system, so an instant investment does make profit according to these calculations.

Now, if an investor would not be interested in an instant investment it is advised to wait until the end of the lifetime of the current system. And afterwards to purchase a CRHP instead of a VCHP. Because the yearly energy cost of a CRHP at $\Delta T_{min} = 3.22$ K is 23 % lower than of a VCHP and the investment cost is not expected to differ much between the two options.

$$\frac{C_{elCRHP}^{p.a.}}{C_{elVCHP}^{p.a.}} = 0.77 \quad (5.9)$$

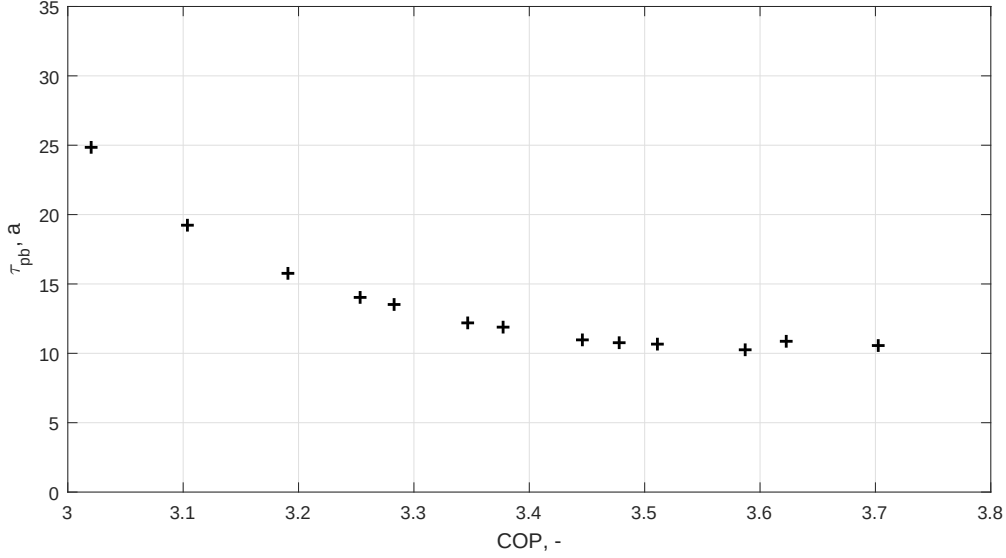


Figure 5.4: Pay-back time

5.2 Concepts for resorber improvement

The total entropy production of the resorber is fixed. At least, under the given application conditions (see figure 1.2) and cycle conditions (see table 3.2), where the minimum temperature difference in the heat exchangers is assumed to be 5 K. When this temperature difference is decreased the entropy production always decreases (see figure 5.1) and the COP increases. The total entropy production is determined by the rate balance of equation (3.3). For convenience it is repeated here:

$$\text{Resorber} : \dot{\sigma} = \dot{m}_R(s_3 - s_2) + \dot{m}_H(s_{H_{out}} - s_{H_{in}}) \quad (5.10)$$

In the resorber model of *chapter 4* the input parameters of equation (5.10) are fixed, and they are used to calculate the heat exchanger area that corresponds to the given operating conditions. There are insufficient degrees of freedom to reduce the entropy production of the resorber. However, measures can be suggested to reduce the area of the resorber. This is the target of improvement in this section.

To reduce the area of the resorber the entropy production rate distribution can be of use. In *chapter 2* equipartition of entropy was treated. It was suggested that a uniformly distributed entropy production will lead to a lower total entropy production. Tondeur and Kvaalen [39] also dealt with the situation of fixed total entropy production. They derived mathematically with the theory of non-equilibrium thermodynamics that for a given duty and given total entropy production the required area is smaller in an equipartitioned configuration than in other configurations. The resorber model of *chapter 4* showed the local entropy production in the resorber (see figure 4.13). The entropy production rate is not near uniformly distributed. A high peak of entropy production occurs in the first 20 % of the heat exchanger area. As was derived previously, the entropy production rate in a single phase fluid that transfers heat depends greatly on the temperature gradients in x-direction. For example for the liquid, combining equations (4.2) and (4.3). The temperature gradients in x-direction depend on the temperature differences between different nodes. For the liquid the temperature gradient is determined by the difference between T^l and T^{Wo} . In the beginning of the process these differences are large and thus the entropy production rate is large there. Some concepts of new configurations of the heat exchangers are presented in the following sections.

5.2.1 Stages

A new configuration is suggested that may possibly increase the uniformity of the entropy production in the resorber. The concept is to divide the process into stages. Starting in the first stage with a small mass flow and in each next stage adding new hot vapour to the working fluid until the original

mass flow is reached. Figure 5.5 shows a schematic representation of this new configuration when the resorption process is divided into seven stages.

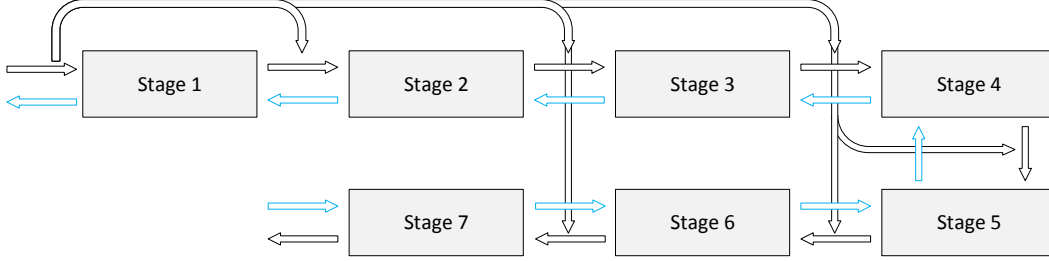


Figure 5.5: Schematic representation of the resorber configuration of seven stages.

The mass flows that are added after each stage are divided into equal portions. The functionality of mixing is added to the resorber model of *chapter 4*, but no entropy production of mixing is considered. When mixing occurs the new concentrations and enthalpies of the vapour are evaluated. The liquid is not directly affected by the addition of vapour. The new concentration in the vapour is determined with a mass balance.

$$X_a^v = \frac{\dot{m}^v X_a^v + \dot{m}_{stage} X_{a,init}^v}{\dot{m}^v + \dot{m}_{stage}} \quad (5.11)$$

Where $X_{a,init}$ is the initial concentration of the vapour and $\dot{m}_{stage}$ is the amount of mass flow that is added after each stage. The new enthalpy of the vapour is:

$$h^v = \frac{\dot{m}^v h^v + \dot{m}_{stage} h_{init}^v}{\dot{m}^v + \dot{m}_{stage}} \quad (5.12)$$

Where h_{init}^v is the initial enthalpy of the vapour. With the new concentration and enthalpy values other properties of the vapour can be obtained, such as temperature and density. The liquid properties are indirectly influenced, because the driving force for transfer over the interface has changed, which results in different exchange rates of heat and mass to the liquid.

The model is run with the inputs of table 4.2, only with $N_p = 5000$ and $\dot{m}_R = 1.5$ kg/s. The mass flow that was added after each stage is equal to $\dot{m}_{stages} = \dot{m}_R$. Figure 5.6 shows the mass flows along the plate length. The red line shows the mass flow of the vapour; each discontinuity indicates that some hot vapour is added. The threshold for mixing to occur is when the quality of the working fluid reaches 0.5 kg/kg. Every time that the red line touches the dark-blue line, a new stage has been reached. This is when the mass of vapour and liquid are equal in the working fluid, so the quality is 0.5 kg/kg. After seven stages the process proceeds beyond $q_{wf} = 0.5$. At the end of the transfer area the process has not finished yet; there is still vapour in the working fluid. More area is required to complete the process of resorption for the application.

Figure 5.7 depicts the local entropy production in the heat exchanger along the length of the plate. It can be observed that the peak in general has spread, compared to the peak in figure 4.13. Unfortunately, the large discontinuities make the local entropy production less uniform. Entropy production of mixing is not taken into account in the calculations; it is expected that this would enlarge the discontinuities of the local entropy production.

It can be concluded that this configuration has a negative effect on the size of the heat exchanger and should not be implemented for that reason. Following the theory of Tondeur and Kvaalen [39], the increase of area can be ascribed to the discontinuities of the local entropy production.

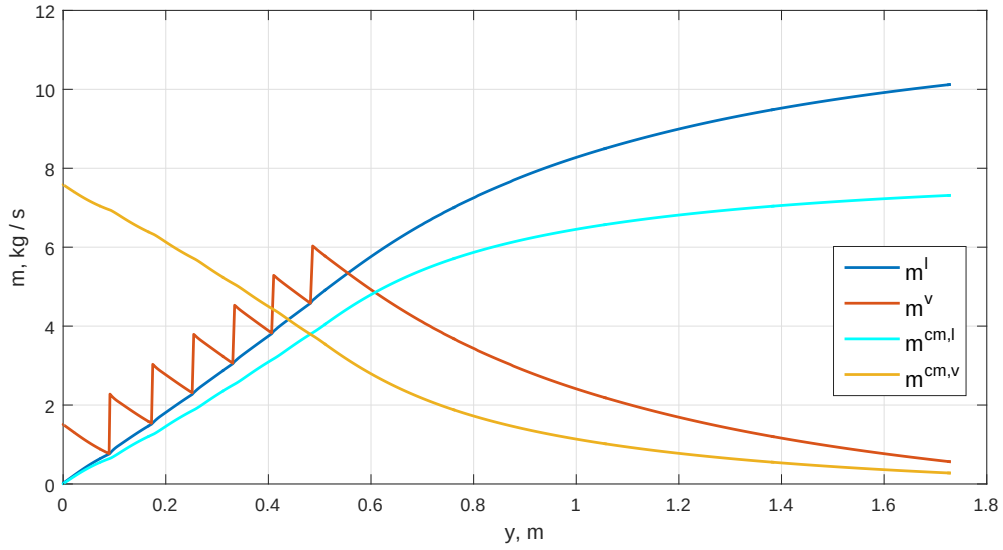


Figure 5.6: Mass flows along the plate length.

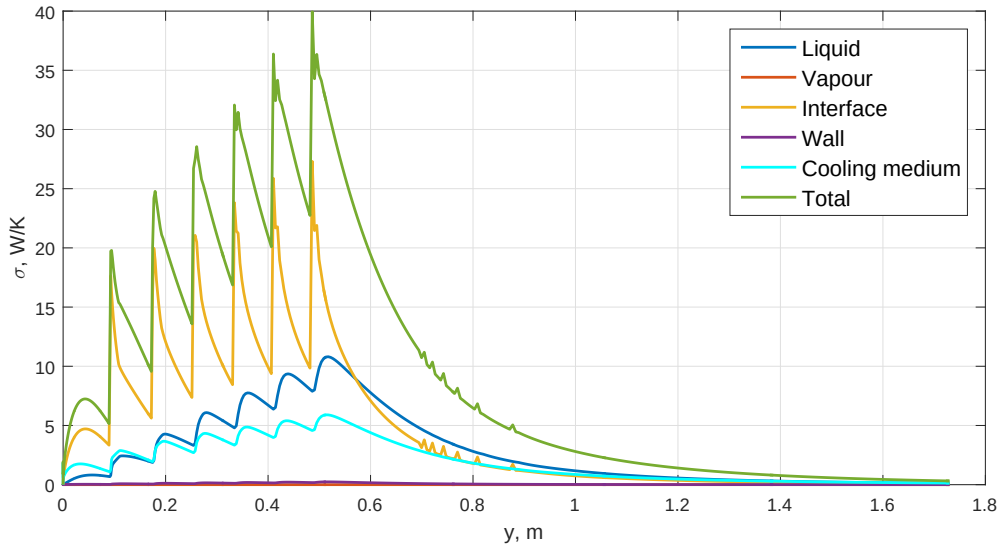


Figure 5.7: Local entropy production along the plate length.

5.2.2 Continuous vapour addition

The next concept that is investigated is continuous vapour mass flow addition. It is the same principle as the concept of stages, only the mass is added slowly and not in such large amounts at the same time. It is expected that the discontinuities in the local entropy production will not appear. Figure 5.8 shows a schematic representation of a plate, which is designed to create this situation. The hot vapour that enters the heat exchanger at the top right inlet is divided into a part (one third) that enters the heat exchanging surface directly and a part (two thirds) that is lead beside the plate. The part that is lead beside the plate is added to the heat exchanging surface along the side of the plate. Probably, practical difficulties will arise when actual design of such a heat exchanger is performed. The separation of the vapour at the inlet might be unsteady. It might be hard to ensure that addition of the vapour along the side of the plate is evenly distributed. Temperature and concentration differences along the width of the plate will occur. These difficulties are neglected for now, and the resorber model of *chapter 4* is

used to find out how the area of the heat exchanger will be influenced in an ideal case. From 10 % to 90 % of the transfer area the mass flow is added in each cell according to the mixing rules of equations (5.11) and (5.12).

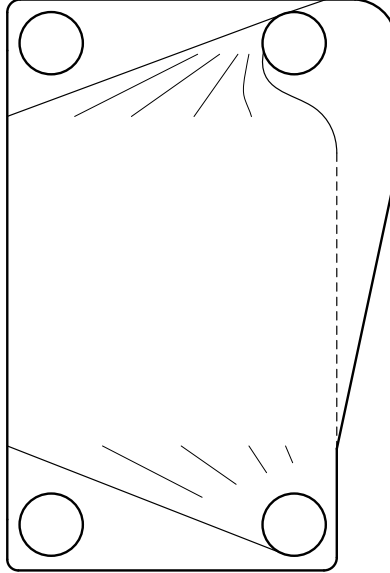


Figure 5.8: Schematic representation of a plate of a plate heat exchanger designed for continuous vapour addition.

The model is run with the inputs of table 4.2, only with $N_p = 5000$ and $\dot{m}_R = 3.6 \text{ kg/s}$. The rest of the vapour mass flow (7.1 kg/s) was added after 10 % of the plate length with a rate of 4.1 kg/s per meter of the plate length. All the vapour has entered the heat exchanging surface at 90 % of the plate length. Figure 5.9 shows the mass flows along the plate length. The red line represents the mass flow of the vapour. There are no discontinuities any more, because the vapour is added in very small amounts. From the very steady increase of the liquid mass flow (constant slope of blue line) after about 0.4 m, it can already be observed that the forces and fluxes are more or less constant. This results in a more uniform distribution of entropy production.

Figure 5.10 shows the local entropy production rate along the plate length. And indeed it is very regular after about 0.4 m. When this figure is compared to figure 4.13 it is clear that the entropy is more evenly distributed in this case than in the example of *chapter 4*. Also the peak in the beginning is significantly smaller.

Unfortunately, as in the previous concept proposal, the process has not completely occurred yet and the area of the resorber should be increased to let it do so. So the measure of continuously vapour addition increases the required area of the heat exchanger. According to Tondeur and Kvaalen [39] a uniform distribution of entropy production leads to lower heat exchanger area, when the duty and the total entropy production is constant. These concepts were proposed assuming that the duration, t , of the process in the heat exchangers would remain constant. This is a condition for the principle of Tondeur and Kvaalen [39] to be true. However, the time is not constant, because the changing mass flow of the working fluid along the length of the heat exchanger causes the velocity of the fluid to change. And this leads to a change of the duration of the process. The effect of continuous addition of hot vapour on the process is a more uniform distribution of entropy production and a decreased duration of the process. The effect on the time of the process was stronger, so that the required area of the heat exchanger increased.

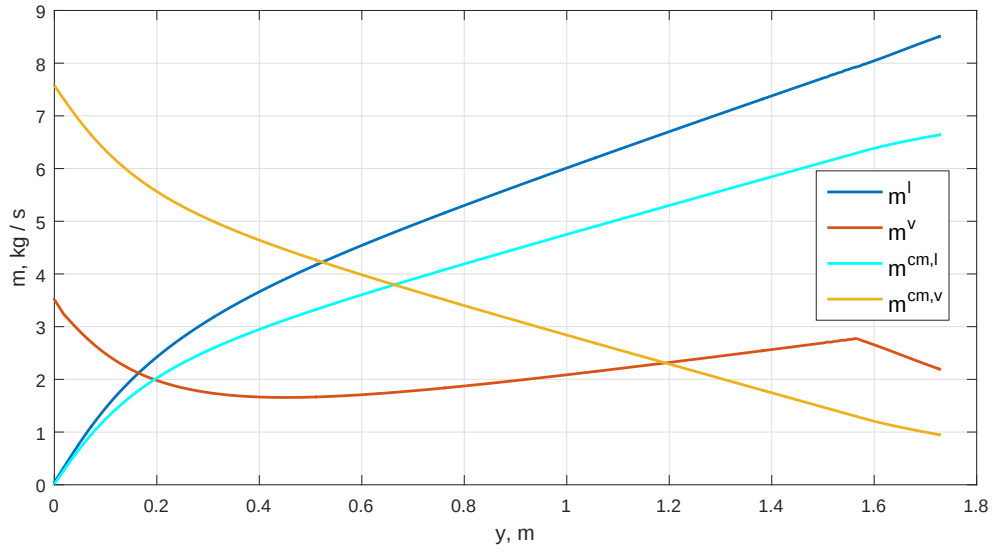


Figure 5.9: Mass flows along the plate length.

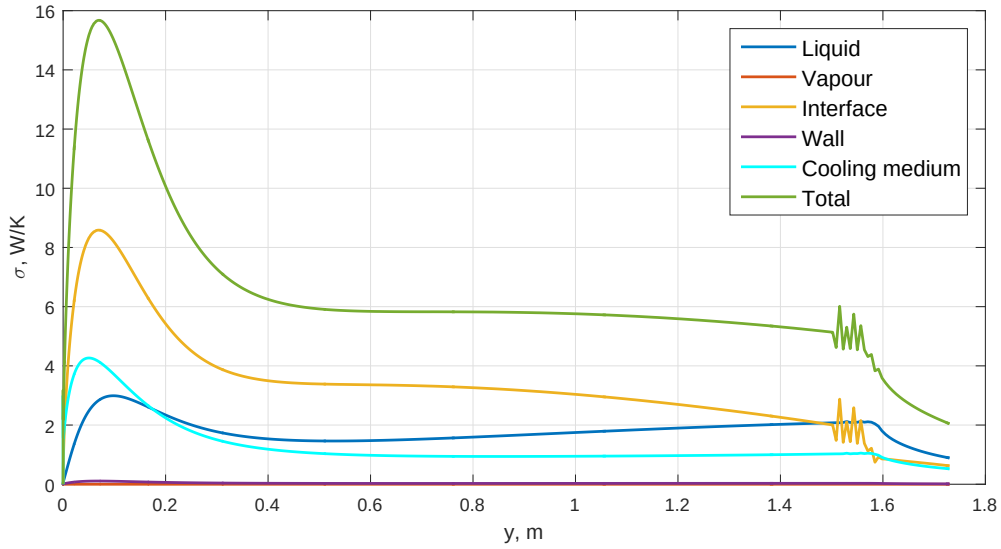


Figure 5.10: Local entropy production along the plate length.

5.2.3 Adjusting cross-sectional area between the plates

The time of a process is of importance in many processes, because it often determines the production of something. In a heat pump cycle the time that the working fluid needs to pass through a component has no effect on the performance. It is proposed to turn around the principle that was used in the previous sections. Now, the configuration of the heat exchanger is kept unchanged and the duration of the process is sought to be increased in order to decrease the area of the heat exchanger. The time that the mass of the working fluid needs to pass through a heat exchanger depends on the velocity of the fluid. The velocity of the fluid can be calculated with:

$$v = \frac{\dot{m}}{\rho A} \quad (5.13)$$

Here A is the cross-sectional area of the flow direction of the mass. The variables of this equation are in a considerable degree subject to variation throughout the process. The vapour and the liquid

of the working fluid have different mass flows, densities and cross-sectional areas, so they will have different velocities. If the total working fluid is considered, the mass flow and the cross-sectional area are constant. The mean density of the two-phase mixture changes along the length of the plate, but it always starts and finishes at the same point. The mass flow is given, but the cross sectional area of the heat exchanger can be adjusted. When the area is increased, the velocity will be decreased and that will cause the duration, t , of the process to increase. The cross-sectional area is determined by:

$$A = W_p \delta_p \quad (5.14)$$

So the width of the plate and the plate spacing should be increased in order to decrease the heat exchanger area. The resorber model is run with a high and low value for W_p and d_p separately. In table 5.2 the results are shown of these adjustments. The first entry corresponds to the result of the example in *chapter 4* and this case is used as a reference here. When the width of the plate is changed, then also the length of the plates changes, because the area of the plate is kept constant. The quality of the working fluid is given at a certain position along the y-axis of the plate. When the quality is zero or near zero below 99 % of the plate length, then the process has finished before all the available plate area was passed. This means that less area is required. When the quality of the working fluid is above zero at the end of the plate, then the process has not completed. In this case more area is required to finish the process. Four cases are evaluated.

First, the width of the plate is changed from 0.75 m to the highest value in the range that is indicated in table 4.1, which is $W_p = \sqrt{A_p/2} = 0.81$ m. All other inputs are kept equal to what was used in the example in *chapter 4*. The result in table 5.2 shows that the difference with the result of the reference situation is very small. It seems that the process has completed before end of the plate. This confirms the expectation.

Next, the plate spacing is changed from 4 mm to the highest value in the range that is indicated in table 4.1, which is $\delta_p = 5$ mm. All other inputs are kept equal to what was used in the example in *chapter 4*. Unfortunately, at the end of the plate there is still vapour in the mixture. This means that the process has not completed and thus requires a larger heat transfer area.

Table 5.2: Evaluation of different plate widths and plate spacings.

W_p , m	δ_p , mm	L_p , m	q_{wf} , kg/kg	Δp , Pa
0.75	4	1.73	0.01 at $y = 0.99L_p$	0.60
0.81	4	1.60	0.00 at $y = 0.98L_p$	0.51
0.75	5	1.73	0.05 at $y = 0.99L_p$	0.35
0.66	4	1.97	0.00 at $y = 0.94L_p$	0.78
0.75	2	1.73	0.01 at $y = 0.46L_p$	2.36

It is thought that in the derivation of Tondeur and Kvaalen [39] it is assumed that the equipment size is not a function of the the contact time. However, a shorter contact time implies a higher velocity of the fluid. The velocity of the fluid increases the heat and mass transfer coefficients that govern the exchange of heat and mass in the process of condensation. Now the cross-sectional area in the flow direction of the heat exchanger will be decreased. Equation (5.13) shows that the velocity of the fluid will then increase. It is expected that the higher velocity of the fluid will have a positive effect on the exchange rates in the process and thus decrease the required heat transfer area.

The width of the plate is changed from 0.75 m to the lowest value in the range that is indicated in table 4.1, which is $W_p = \sqrt{A_p/3}$. Other input values were taken as in table 4.1. The result in table 5.2 shows that the vapour has condensed before the end of the plate.

At last, the plate spacing is changed from 4 mm to 2 mm. Unfortunately, the plate spacing could not be brought lower, because the model experienced difficulties in the calculation. Other input values were taken as in the example of *chapter 4*. The result in table 5.2 shows that the influence of the plate spacing is large.

The pressure drop is also calculated with the correlations that were previously presented. In table 5.2 the results are shown of the method of Yan et al. [42] for the different cases. The characteristics of the flow do not lie within the ranges that this correlation is appropriate for. Therefore the quantitative results only give a rough indication of the order of magnitude, which is small. As the cross-sectional area is decreased, the pressure drop increases. This should be expected, regarding the influence of δ_p and W_p on the mass flux $\dot{G}$ and the hydraulic diameter d_h in the pressure drop correlations.

Figure 5.11 depicts the mass flows of vapour for the five different cases along the dimensionless plate length. This graph provides insight into the progress of the process of condensation in the heat exchanger. The blue line corresponds to the reference situation. The red line has a discontinuity at around 53 % of the plate length. This is caused by an error in the energy balance iteration, see figure 4.3. If this error had not occurred, then the red line would have continued more or less parallel to the blue one. Then it would have ended above the reference line and this would indicate that the process requires more area to finish. Figure 5.12 presents the vapour-interface heat transfer coefficients for the

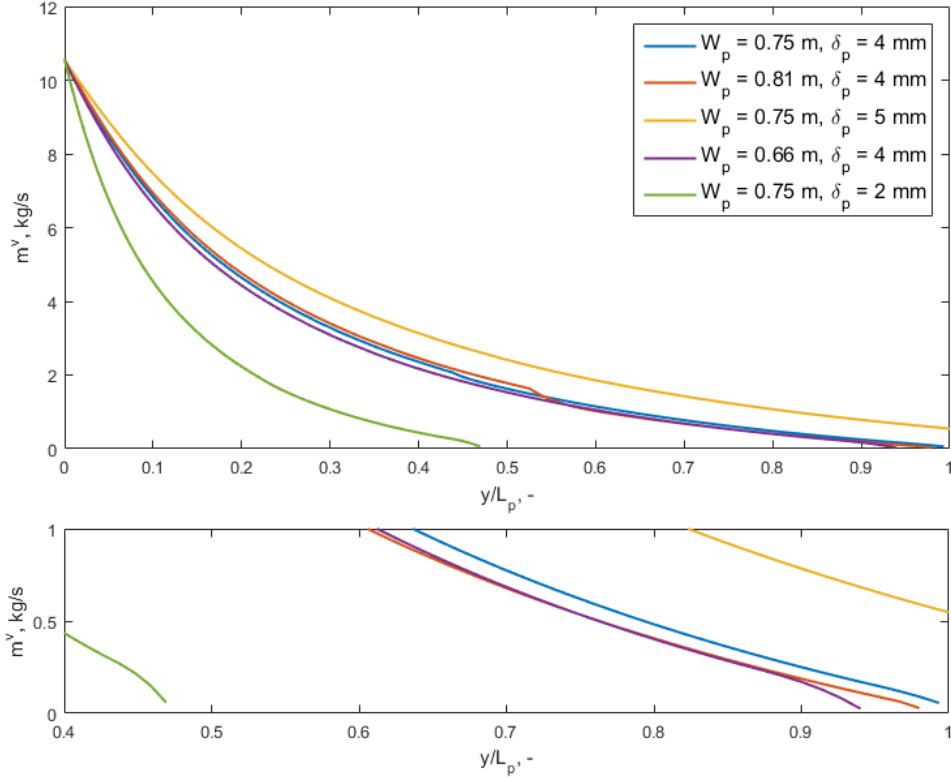


Figure 5.11: Vapour mass flows along the dimensionless plate length where the plate width and plate spacings have been adjusted.

different cases along the dimensionless plate length. They were obtained with the correlation of Seader and Henley [35] (equation (4.60)). The heat transfer coefficients determine the degree of influence of the forces on the fluxes of heat exchange. Transfer coefficients are the inverse of resistivity coefficients, see equation (2.14). Especially when the forces are high, the transfer coefficients play an important role to determine the fluxes. The forces are high in the first part of the resorber, therefore a close-up is shown of this part in figure 5.12.

These results confirm the idea that with a given duty, a given total entropy production and a constant entropy production distribution, a decreased cross-sectional area in the flow direction leads to higher velocities and higher exchange rates and thus a smaller heat exchanger area. The limit of this measure will be determined by the pressure drop that is accepted for a certain application.

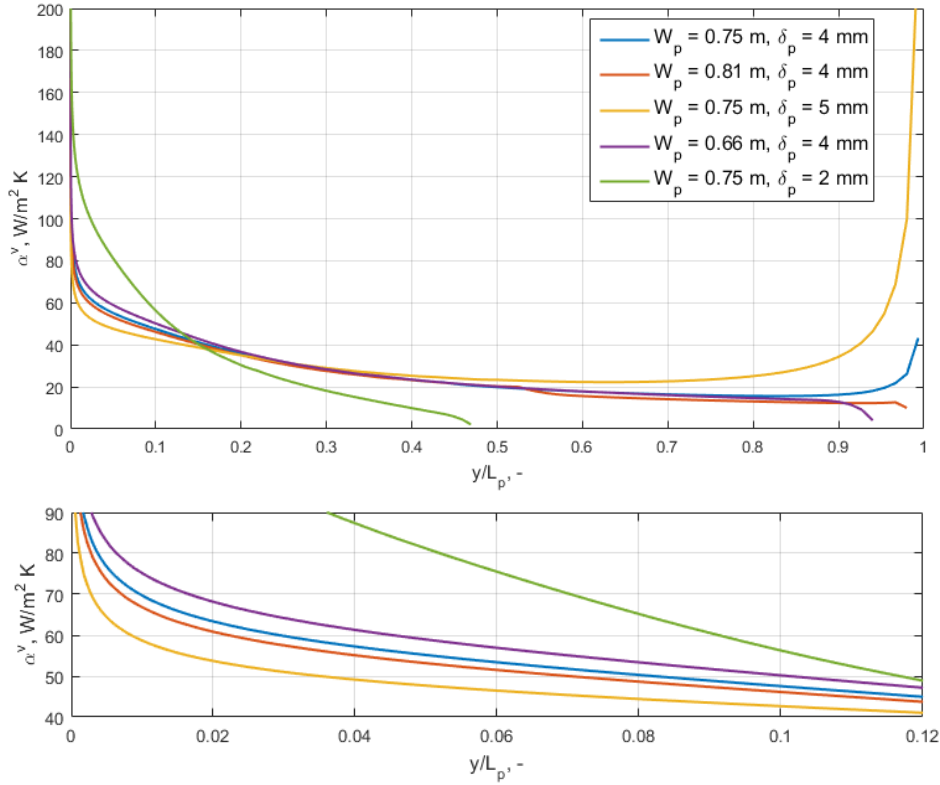


Figure 5.12: Heat transfer coefficient in the film along the dimensionless plate length where the plate width and plate spacings have been adjusted.

5.3 Model discussion

The models that have been developed have some weaknesses that should be acknowledged to be able to judge the reliability of the results in some measure. Two models have been developed; a cycle performance model and a resorber model. The most important issue is that the models have not been validated with experiments.

Further a number of issues will be dealt with concerning the resorber model of *chapter 4*.

- Laminar and steady flow of the film along the wall is considered. In reality the film might be wavy or even turbulent. Then the interface boundary becomes unclear and the film thickness is unsteady. There are no different flow regimes considered in the working fluid. Fernández-Seara et al. [13] did consider different flow regimes, but that was in a bubble absorber. This consideration influences the choice of transfer correlations.
- The two-film theory of Whitman is assumed. This means that mass diffusion is neglected in the vapour bulk and the liquid bulk of the working fluid. Therefore all the mass transfer occurs in the interfacial region. This impacts the way in which the entropy production is calculated.
- The modelling equations of the thermodynamic state model only apply when both vapour mass and liquid mass are present in the system. At the inlet of the resorber, where there is only vapour, the model does not work. Therefore it is assumed that 1 % of the vapour mass has condensed already at the inlet of the resorber.
- Frictional pressure drop has been taken into account. Yan et al. [42] pointed out that in their case the frictional pressure drop accounted for more than 93 % of the total pressure drop. However, it is expected that there will be a significant pressure drop due to contraction and expansion through the ports of the plate heat exchanger in the considered application. Because Sinnott and Towler [37] indicate that this pressure drop contribution is proportional to the number of channels, which is large for the considered application.

- The transfer correlations that were used for the heat transfer and pressure drop have certain ranges for which they are valid. These conditions are not always satisfied in the calculations. For instance for the cooling medium transfer coefficient α^{cm} in the example of *chapter 4* according to the method of Amalfi et al. [3], β_r , $Re^{cm,v}$ and Bd are within the range, but ρ_r and Bo are too high and $Re^{cm,lo}$ is too low. And together this causes Nu to be too low (equation (4.49)).
- The liquid Reynolds number has been calculated with the vapour density instead of the liquid density. This is an error in the model. The density is used to determine the velocity v^l for equation (4.61). This error influences the liquid-interface heat transfer coefficient α^l . Figure 5.13 shows three different transfer coefficients. α_{corr}^l is the corrected coefficient which uses the liquid density correctly for the Reynolds number in the correlation of Seader and Henley [35]. As can be seen in the figure the difference between α^l and α_{corr}^l is significant. As was mentioned previously the α^l can also be taken to be equal to α^f as was done by Fernández-Seara et al. [14]. For comparison the heat transfer coefficient of the film α^f is also shown in figure 5.13.

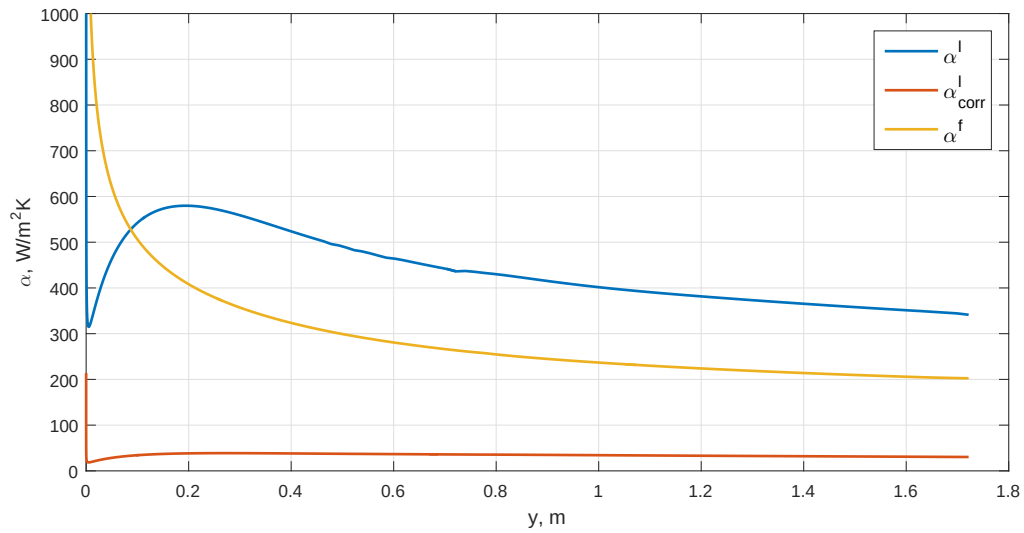


Figure 5.13: Heat transfer coefficients along the length of the plate.

Chapter 6

Conclusions and recommendations

The objective of this research was to find the most energy efficient performance of a compression-resorption heat pump keeping the payback time under three years. The *COP* of the system is the measure for the energetic performance of a heat pump. The economical profit of the new system is defined by the saving of energy cost with respect to the currently installed system.

- A payback time of three years is not attainable for a CRHP for the considered the application. The shortest payback time is 10.28 years. The optimised *COP* of the system is then 3.6 (entropy production is minimised). The shortest payback time is still shorter than the lifetime of the system (15 years), so an instant investment still is profitable.

A literature study and two models were developed that contribute to the objective. A cycle performance model and a detailed model of the resorber were constructed. Furthermore, the resorber model was adjusted to investigate alternative configurations of the heat exchangers. The following conclusions can be drawn from the cycle performance model from *chapter 3*:

- The optimal ammonia concentration of the CRHP with an ammonia-water mixture in the considered application is 0.7 mol/mol . At this concentration the total entropy production of the system is minimal.
- The highest *COP* of the CRHP is 3.48. This is higher than any of the other considered alternatives (see table 3.3). The minimum temperature difference in the resorber was kept above 5 K, otherwise an even higher *COP* is attainable.
- The resorber is the component with the largest entropy production (44.6 %). This is caused by the poor match of the temperature profiles of the working fluid and the application fluid.
- The best working fluid that should be used in a VCHP for the considered application is acetone. It leads to the highest *COP* with an acceptable pressure at the inlet of the compressor (above 0.3 bar). This alternative approaches the optimal performance of a CRHP (see table 3.3 and appendix A).

A detailed model was developed for the resorber, because it was shown to be the component with the highest losses. The following conclusions can be deduced from the results of this model:

- The entropy production rate in the resorber is not near uniformly distributed. It is high at the beginning when the forces for heat transfer and mass transfer are high (see figure 4.13).
- In the example with the input conditions of table 4.2 the required heat exchanger area was 5525 m^2 . For this eleven full size heat exchangers of 500 m^2 are required and one additional smaller one.

A feasibility study was carried out and presented in *chapter 5*. The investment cost of the heat exchangers and the compressor were calculated and the energy cost of the system over a lifetime of fifteen years. Also the payback period was determined, where the profit was defined to be the cost saving of the CRHP with respect to the currently installed VCHP.

- The cheapest option for the installation of the CRHP has a *COP* of 3.7, see figure 5.3. The investment cost is 9.1 M€, the energy cost over the lifetime of the system of fifteen years is 37.7 M€ and the payback period is 10.57 years.

- The shortest payback time is 10.28 years. In this case the COP of the system is 3.6. And the total cost becomes 46.9 M€.

Also in *chapter 5* the resorber model was adjusted to investigate alternative heat exchanger configurations. A reduction of the heat exchanger area was the target of the alternatives. From these investigations it can be concluded that:

- The concept of stages causes the area of the resorber to increase. Discontinuities are introduced in the local entropy production so that it becomes even less uniform along the length of the plate of the heat exchanger.
- The concept of continuous vapour addition also increases the required area of the resorber. The entropy production rate has become more uniform. However, it would only positively affect the required area if the duration of the process would have been kept constant. And that was not the case.
- A reduction of the cross-sectional area of the flow direction in the heat exchanger causes the required heat exchanger area to decrease. To reduce this area the plate spacing and the width of the plate can be decreased.

This study will be concluded with some recommendations regarding the feasibility of the application and further research.

- If an investor would not be interested in an instant investment it is advised to wait until the end of the lifetime of the currently installed system. And afterwards to install a CRHP instead of a new VCHP. Because the yearly energy cost of a CRHP at $\Delta T_{min} = 3.22$ K is 23 % lower than of a VCHP. The investment cost is not expected to differ much between the two options. 23 % less compressor power is required for the same duty; when this would be applied on a large scale it would significantly contribute to the goal of the European Council [12] to improve energy efficiency by 27 % in 2030.
- The results of both models that have been developed should be validated with experiments. For validation of the cycle model an actual CRHP cycle with ammonia-water as working fluid should be installed. Perhaps on a laboratory scale at first. For validation of the resorber model a setup should be prepared for a plate heat exchanger with ammonia water as hot fluid and water as cold fluid. Measurements should be performed not only at the in- and outlet of the heat exchanger, but also along the length of the plates.
- Investigate the effect of the heat losses to the environment. For both models this is interesting. The COP of the cycle will decrease when this effect is taken into account, but how much will the difference be?
- The resorber model can be adjusted in order to use it for the desorber quite easily. If accurate calculations of the desorber area are desired this is certainly a good approach.
- With regard to the performance of the CRHP priority must be given to the improvement of the efficiency of wet compression. In this work the isentropic efficiency is assumed to be 70 %. If it were only 60 % the CRHP would perform worse than a conventional VCHP with acetone (see table 3.3). To the knowledge of the author neither of these efficiencies have been achieved in practice yet.
- Innovative configurations of the heat exchangers may be sought after to increase the uniformity of the distribution of the entropy production rate. Such a configuration will only cause the required area to decrease when the duration of the process is unchanged.

Appendix A

Vapour-compression heat pump performance

In this appendix the results of a cycle performance model of a VCHP are presented. For the calculations the property database of Refprop [24] is used. The isentropic efficiency of the compressor is assumed to be 70 %. The fluid is condensed to saturated liquid in the condenser and evaporated to saturated vapour in the evaporator. It is assumed that there are no heat losses to the environment and no pressure drops in heat exchangers and pipes. Table A.1 shows the coefficient of performance of the same heat pump with different working fluids. The calculations were performed for all the available fluids from the Refprop database [24], but only the 50 fluids with the best performance are ordered and shown. The pressure in the evaporator, $p_{4,1}$, must be above 0.3 bar to ensure safe operation of the compressor. The maximum discharge pressure, $p_{2,3}$, for a screw compressor is around 1100 psig [15], which is 75 bar. Taking this into account, the cycle has the best performance with acetone as working fluid.

Table A.1: Performance results of a vapour-compression heat pump with different working fluids integrated in the application.

Working fluid	$p_{4,1}$, bar	$p_{2,3}$, bar	$\dot{m}_C$, kg/s	COP , -	Working fluid	$p_{4,1}$, bar	$p_{2,3}$, bar	$\dot{m}_C$, kg/s	COP , -
ethanol	0.14	3.03	52.1	3.40	undecane	0.00	0.06	48.3	2.90
methanol	0.28	4.66	52.1	3.39	nonane	0.01	0.29	48.3	2.89
benzene	0.20	2.28	51.4	3.30	R123	1.31	9.56	48.3	2.89
acetone	0.47	4.66	51.4	3.29	octane	0.03	0.62	48.2	2.89
toluene	0.06	0.97	51.3	3.27	ammonia	13.51	74.37	48.1	2.87
dihydroxyacetone	0.12	1.79	51.2	3.26	heptane	0.10	1.37	48.1	2.87
ethylbenzene	0.02	0.46	50.9	3.23	hexane	0.31	3.08	47.8	2.84
water	0.06	1.39	50.4	3.15	c-C4H8	2.91	16.90	47.7	2.83
heavy water	0.05	1.33	50.4	3.15	ether	1.03	8.00	47.3	2.79
cyclopentane	0.62	5.12	50.4	3.15	pentane	0.98	7.22	47.1	2.76
hexene	0.20	2.21	50.2	3.12	R1233ZD	1.83	12.62	47.0	2.76
R21	2.53	15.94	50.2	3.12	2-methylpentane	0.42	3.83	47.0	2.76
R11	1.49	9.94	50.1	3.11	t-C4H18	3.17	17.94	46.7	2.72
sulfur dioxide	5.42	33.29	49.8	3.07	R245ca	1.45	11.39	46.5	2.70
R141b	1.12	8.24	49.8	3.07	i-C8H18	0.10	1.33	46.4	2.69
CGP-7930	0.00	0.00	49.7	3.06	i-C5H12	1.29	8.72	46.2	2.67
heptene	0.10	1.27	49.4	3.03	cyclopropene	7.70	39.48	46.2	2.67
nonene	0.01	0.25	49.3	3.01	C4H5F5	0.84	7.25	45.8	2.64
methyl linoleate	0.00	0.00	48.8	2.95	butene	3.98	21.14	45.5	2.60
R40	7.64	38.15	48.8	2.95	R245fa	2.12	15.37	45.1	2.57
heptadecanoic acid	0.00	0.00	48.7	2.94	R142b	4.54	24.60	45.1	2.57
methyl oleate	0.00	0.00	48.7	2.94	dimethyl ether	7.80	38.76	44.8	2.54
R113	0.65	5.37	48.4	2.90	i-C4H8	4.08	21.66	44.8	2.54
dodecane	0.00	0.03	48.3	2.90	butane	3.28	18.12	44.8	2.54
decane	0.00	0.14	48.3	2.90	propene	9.40	42.64	44.7	2.54

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List of Symbols

Roman symbols

A	Area, m^2
a	Amplitude of plate wave / Cost constant for intercept, m , $-$
b	Cost constant for slope, $-$
Bo	Boiling number, $-$
Bd	Bond number, $-$
C	Cost, €
c	Molar concentration / Specific cost, mol mol^{-1} , € kWh^{-1}
COP	Coefficient of performance, $-$
c_p	Specific heat capacity at constant pressure, $\text{J kg}^{-1} \text{K}^{-1}$
D	Diffusion coefficient, $\text{m}^2 \text{s}^{-1}$
d	Diameter, m
$\dot{E}$	Exergy flow rate, W
F	Mass transfer coefficient, $\text{mol s}^{-1} \text{m}^{-2}$
f	Factor, $-$
$\dot{G}$	Mass flux, $\text{kg s}^{-1} \text{m}^{-2}$
g	Gravitational acceleration, m s^{-2}
h	Specific enthalpy, kJ kg^{-1}
i	Counter, $-$
J	Flux, rate m^{-2}
j	Friction factor, $-$
k	Number, $-$
L	Length, m
$\dot{m}$	Mass flow, kg s^{-1}
M	Molar mass, kg mol^{-1}
$\dot{n}$	Molar flow rate, mol s^{-1}
N	Number, $-$
n	Number / Cost constant for exponent, $-$, $-$
Nu	Nusselt number, $-$
p	Pressure, Pa
Pr	Prandtl number, $-$
$\dot{Q}$	Heat transfer rate, W
q	Vapour quality, $-$
R	Phenomenological resistivity coefficient / Universal gas constant, $-$, $\text{J K}^{-1} \text{mol}^{-1}$
Re	Reynolds number, $-$
S	Entropy / Size parameter, J K^{-1} , $-$
s	Specific entropy, $\text{J kg}^{-1} \text{K}^{-1}$
Sc	Schmidt number, $-$
$\bar{T}$	Thermodynamic averaged temperature, K
T	Temperature, K
t	Time, s
U	Overall heat transfer coefficient, $\text{W m}^{-2} \text{K}^{-1}$
V	Volume, m^3
v	Specific volume, $\text{m}^3 \text{kg}^{-1}$ / Velocity, m s^{-1}

$\dot{W}$	Work, W
W	Width, m
X	Driving force / Mass concentration / Wave number, $-, kg\,kg^{-1}, -$
x	Length coordinate perpendicular to flow direction, m
y	Length coordinate in flow direction, m
z	Molar flux ratio (ammonia to total), $-$

Greek symbols

α	Heat transfer coefficient, $W\,m^{-2}\,K^{-1}$
β	Chevron angle, $^{\circ}$
γ	Surface tension, $N\,m^{-1}$
Δ	Difference
δ	Thickness / distance, m
ϵ	Heat transfer correction factor, $-$
η	Efficiency, $-$
Φ	Surface enhancement factor, $-$
ϕ	Fugacity coefficient, $-$
Λ	Wavelength of plate, m
λ	Thermal conductivity, $W\,m^{-1}\,K^{-1}$
μ	Chemical potential / dynamic viscosity, $J\,mol^{-1}, Pa\,s$
∇	Gradient
ν	Kinematic viscosity, $m^2\,s^{-1}$
ρ	Density, $kg\,m^{-3}$
$\dot{\sigma}$	Entropy production rate, $W\,K^{-1}$
τ	Time, a

Sub- and superscripts

'	Measurable
*	Saturated
★	Phase change
0	Reference
II	Second law
a	Ammonia
b	Boundary layer
C	Source (application side)
c	Cell / Compressor
cm	Cooling medium
$corr$	Corrected
cr	Critical
$CRHP$	Related to a compression-resorption heat pump
cur	Currency
d	Destruction
des	Desorber
el	Electric
eq	Equivalent
ev	Source (refrigerant side)
f	Film
H	Sink (application side)
h	Hydraulic
hex	Heat exchanger
i	Interface / Inner / Investment
i, j, k	Number of contribution
in	Inlet
inf	Inflation
$init$	At initial conditions
$inst$	Installation

<i>is</i>	Isentropic
<i>l</i>	Liquid
<i>lo</i>	Liquid only
<i>lost</i>	Lost
<i>life</i>	Life time
<i>lower</i>	Lower limit
<i>max</i>	Maximum
<i>min</i>	Minimum
<i>mol</i>	Molar
<i>m</i>	Mean
<i>o</i>	Outer
<i>out</i>	Outlet
<i>p</i>	Plate
<i>p.a.</i>	Per annum
<i>pb</i>	Payback period
<i>q</i>	Related to heat transfer
<i>R</i>	Refrigerant / working fluid
<i>r</i>	Reduced / ratio
<i>rev</i>	Reversible cycle
<i>stage</i>	Per stage
<i>T</i>	Thermal, evaluated at a constant temperature
<i>total</i>	The sum of the separate parts
<i>tp</i>	Two-phase
<i>upper</i>	Upper limit
<i>V</i>	Per unit volume
<i>v</i>	Vapour
<i>VCHP</i>	Related to a vapour-compression heat pump
<i>W</i>	Wall
<i>w</i>	Water
<i>wf</i>	Working fluid

Abbreviations

CRHP	Compression-resorption heat pump
VCHP	Vapour-compression heat pump
ref.	Reference