Optimal operation of an Ammonia refrigeration cycle

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1 Introduction

Cyclic processes for heating and cooling are widely used in many applications and their power ranges from less than 1 kW to above 100 MW. Most of these applications use the vapor compression cycle to “pump” energy from a low to a high temperature level.

The first application, in 1834, was cooling to produce ice for storage of food, which led to the refrigerator found in every home (Nagengast, 1976). Another well-known system is the air-conditioner (A/C). In colder regions a cycle operating in the opposite direction, the “heat pump”, has recently become popular. These two applications have also merged together to give a system able to operate in both heating and cooling mode.

A schematic drawing of a simple cycle is shown in Figure 1 together with a typical pressure-enthalpy diagram for a sub-critical cycle. The way the cycle works:

The low pressure vapour (4) is compressed by supplying work W_s to give a high pressure vapour with high temperature (1). This stream is cooled to the saturation temperature in the first part of the condenser, condensed in the middle part and possibly sub-cooled in the last part to give the liquid (2). In the expansion choke, the pressure is lowered to its original value, resulting in a two-phase mixture (3). This mixture is vaporized and heated through the evaporator giving a super-heated vapour (4) closing the cycle.

The coefficients of performance for a heating cycle (heat pump) and a cooling cycle (refrigerator, A/C) are defined as

$$COP_h = \frac{Q_h}{W_s} = \frac{\dot{n}(h_1 - h_2)}{\dot{n}(h_1 - h_4)} \qquad \text{and} \qquad COP_c = \frac{Q_c}{W_s} = \frac{\dot{n}(h_4 - h_3)}{\dot{n}(h_1 - h_4)} \tag{1}$$

respectively. Heat pumps typically have a COP of around 3 which indicates that 33% of the gained heat is addet as work (eg. electric power).

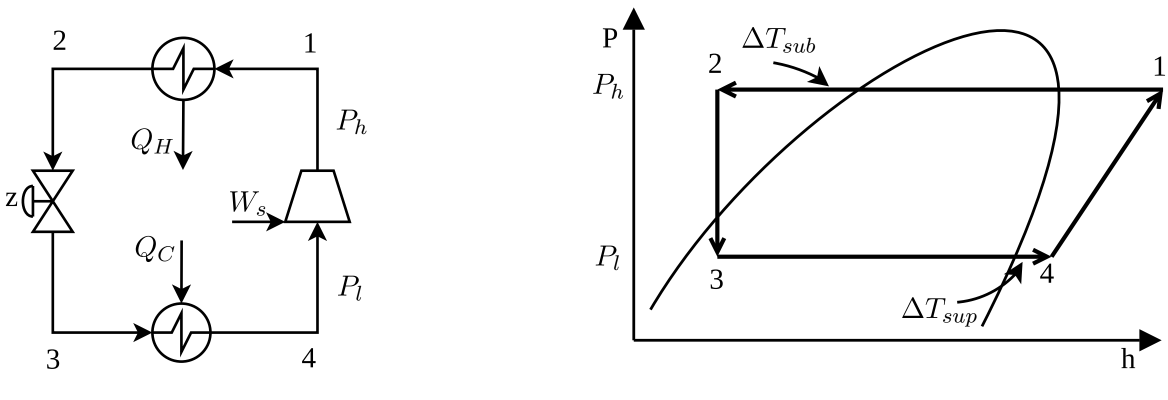


Figure 1: Schematics of a simple vapor compression cycle with typical pressure-enthalpy diagram indicating both sub-cooling and super-heating

In industrial processes, especially in cryogenic processes such as air separation and liquefaction of natural gas (LNG process), more complex cycles are used in order to improve the thermodynamic efficiencies. These modifications lower the temperature differences in the heat exchangers and include cycles with mixed refrigerants, several pressure levels and cascaded cycles. The Mixed Fluid Cascade process developed by the Statoil Linde Technology Alliance is being built at the LNG plant in northern Norway and incorporates all of the above modifications. The resulting plant has three cycles, all with mixed refrigerant and the first with two pressure levels. Our long term objective is to study the operation of such processes. However, as a start we need to understand the simple cycle in Figure 1.

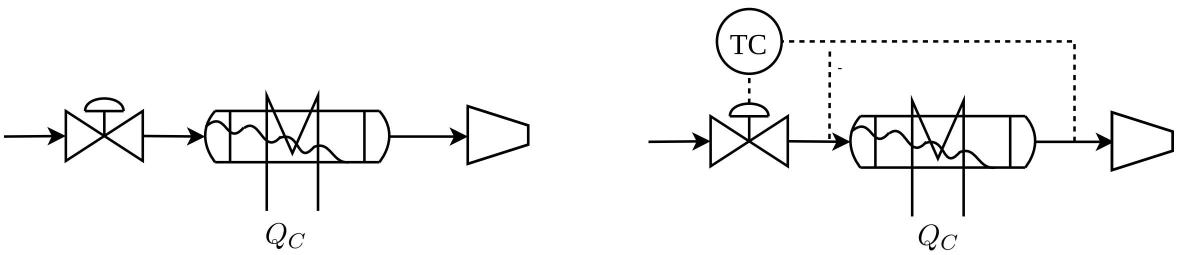
2 Operation of simple vapour compression cycles

2.1 Design versus operation

Table 1 shows typical specifications for simple cycles in design (find equipment) and in operation (given equipment). Note that the five design specifications results in only four equipment parameters; compressor work W_s, valve opening z and UA for the two heat exchangers. As a consequence, with the four equipment parameters specified, there is not a unique solution in terms of the operation. The "un-controlled" mode is related to the pressure level, which is indirectly set by the charge of the system. This is unique for closed systems since there is no boundary condition for pressure. In practice, the "pressure level" is adjusted directly or indirectly, depending on the design, especially of the evaporator. This is considered in more detail below.

Table 1: Specifications in design and operation

	Given	#
Design	Load (e.g. Q_h), P_l, P_h, ΔT_{sup} and ΔT_{sub}	5
Operation	W_s (load), choke valve opening (z) and UA in two heat exchangers	4



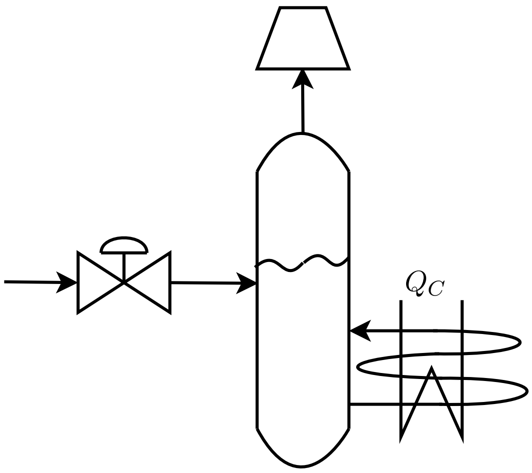
(a) Fixed valve (design I.a)

(b) With thermostatic expansion valve (design I.b)

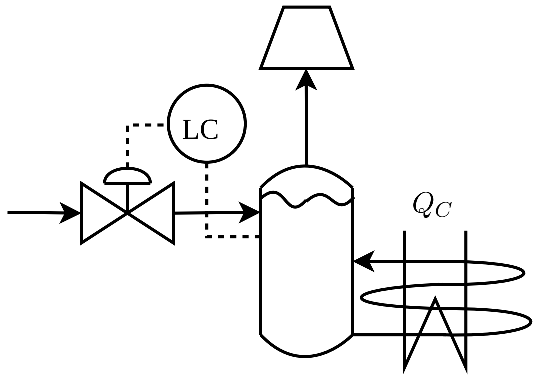
Figure 2: Dry evaporator

2.2 Operational (control) degrees of freedom

During operation the equipment is given. Nevertheless, we have some operational or control degrees of freedom. These include the compressor power (W_s), the charge (amount

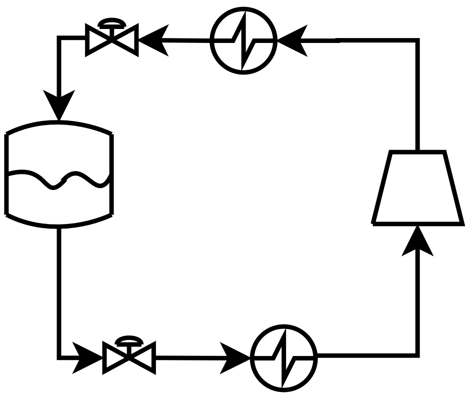


(a) Valve free (design II.a)

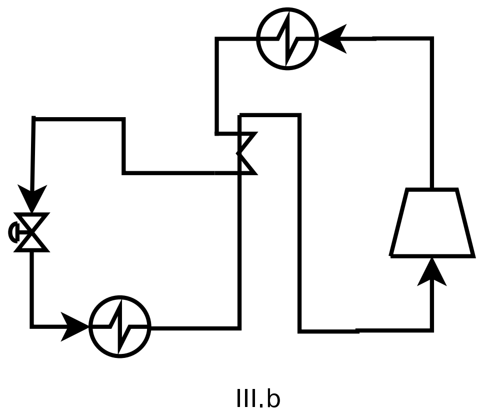


(b) With level control (design I.b)

Figure 3: Flooded evaporator



(a) Design with liquid receiver and extra choke valve (design III.a)



(b) Internal heat exchanger

Figure 4: Liquid receiver (design III.b)

of vapour and liquid in the closed system), and the valve openings. The following valves may be adjusted on-line:

- Adjustable choke valve (z); see Figure 1 (not available in some simple cycles)
- Adjustable valve between condenser and storage tank (for designs with a separate liquid storage tank before the choke; see design III.a in Figure 4(a))

In addition, we might install bypass valves on the condenser and evaporator to effectively reduce UA, but this is not normally used because use of bypass gives suboptimal operation.

Some remarks:

- The compression power W_s sets the "load" for the cycle, but it is otherwise not used for optimization, so in the following we do not consider it as an operational degree of freedom.
- The charge has a steady-state effect for some designs because the pressure level in the system depends on the charge. A typical example is household refrigeration systems. However, such designs are generally undesirable. First, the charge can usually not be adjusted continuously. Second, the operation is sensitive to the initial charge and later to leaks.
- The overall charge has no steady-state effect for some designs. This is when we have a storage tank where the liquid level has no steady-state effect. This includes designs with a liquid storage tank after the condenser (design III.a Figure 4(a)), as well as flooded evaporators with variable liquid level (design II.b Figure 3(a)). For such designs the charge only effects the level in the storage tank. Note that it may be possible to control (adjust) the liquid level for these designs, and this may then be viewed as a way of continuously adjusting the charge to the rest of the system (condenser and evaporator).
- There are two main evaporator designs; the dry evaporator (2) and the flooded evaporator (3). In a dry evaporator, we generally get some super-heating, whereas there is no (or little) super-heating in a flooded evaporator. The latter design is better thermodynamically, because super-heating is undesirable from an efficiency (COP) point of view. In a dry evaporator one would like to control the super-heating, but this is not needed in a flooded evaporator. In addition, as just mentioned, a flooded evaporator with variable liquid level is insensitive to the charge.
- It is also possible to have flooded condensers. and thereby no sub-cooling, but this is not desirable from a thermodynamic point of view.

2.3 Use of the control degrees of freedom

In summary, we are during operation left with the valves as degrees of freedom. These valves should generally be used to optimize the operation, In most cases "optimal operation" is defined as maximizing the efficiency factor, COP. We could then envisage an on-line optimization scheme where one continuously optimizes the operation (maximizes COP) by adjusting the valves. However, such schemes are quite complex and sensitive to uncertainty, so in practice one uses simpler schemes where the valves are used to control some other variable. Such variables could be:

- Valve position setpoint z_s (that is, the valve is left in a constant position)
- High pressure (P_h)

- Low pressure (P_l)
- Temperature out of condenser (T_2) or degree of sub-cooling ($\Delta T_{sub} = T_2 - T_{sat}(P_h)$)
- Temperature out of evaporator (T_4) or degree of super-heating ($\Delta T_{sup} = T_4 - T_{sat}(P_l)$)
- Liquid level in storage tank (to adjust charge to rest of system)

The objective is to achieve "self-optimizing" control where a constant setpoint for the selected variable indirectly leads to near-optimal operation (Skogestad, 2000).

Control (or rather minimization) of the degree of super-heating is useful for dry evaporator with TEV (design II.b Figure 2(b)). However, it consumes a degree of freedom. In order to retain the degree of freedom, we need to add a liquid storage tank after the condenser (design III.a Figure 4(a)). In a flooded evaporator, the super-heating is minimized by design so no control is needed.

With the degree of super-heating fixed (by control or design), there is only one degree of freedom left that needs to be controlled in order to optimize COP. To see this, recall that there are 5 design specifications, so optimizing these give an optimal design. During operation, we assume the load is given (W_s), and that the maximum areas are used in the two heat exchangers (this is optimal). This sets 3 parameters, so with the super-heating controlled, we have one parameter left that effects COP.

In conclusion, we need to set one variable, in addition to ΔT_{sup}, in order to completely specify (and optimize) the operation. This variable could be selected from the above list, but there are also other possibilities. Some common control schemes are discussed in the following.

2.4 Some alternative designs and control schemes

Some designs are here presented and the pro's and con's are summarized in Table 2.

2.4.1 Dry evaporator (I)

For this design there is generally some super-heating.

I.a In residential refrigerators it is common to replace the valve by a capillary tube, which is a small diameter tube designed to give a certain pressure drop. On-off control of the compressor is also common.

I.b Larger systems usually have a thermostatic expansion valve (TEV) , (Dossat, 2002) and (Langley, 2002), that controls the temperature and avoids excessive super-heating. A typical super-heat value is 10 $^\circ C$.

2.4.2 Flooded evaporator (II)

A flooded evaporator differs from the dry evaporator in that it only provides vaporization and no super-heating.

II.b In flooded evaporator systems the valve is used to control the level in either evaporator or condenser (Figure 3(b)).

II.a We propose a design where the volume of the flooded evaporator is so large that there is no need to control the level in one of the heat exchangers. This design retains the valve as a degree of freedom (Figure 3(a)).

2.4.3 Other designs (III)

III.a To reduce the sensitivity to the charge in designs I.b and II.b it is possible to include a liquid receiver before the valve as shown in Figure 4(a). To retain a degree of freedom a valve may be added before the receiver.

III.b It is possible to add an internal heat exchanger as shown in Figure 4(b). This will super-heat the vapor entering the compressor and sub-cool the liquid before expansion. The latter is positive because of reduced expansion losses, whereas the first is undesirable because compressor power increases.

Table 2: Operation of alternative designs

	Pro's	Con's
I.a	Simple design	Sensitive to charge
		No control of super-heating
I.b	Controlled super-heating	Super-heating
		Sensitive to charge
II.a	No super-heating by design	
	Not sensitive to charge	
	Valve is free	How to use valve?
II.b	No super-heating by design	Sensitive to charge
III.a	Not sensitive to charge	Complex design
		How to use valve?

3 Ammonia case study

3.1 System description

The cycle operates between air inside a building ($T_C = T_{room}$) and ambient air ($T_H = T_{amb}$) removing 20 kW of heat (Q_C) from the building. This could be used in a large cold storage building as illustrated in Figure 5.

Thermodynamics: SRK equation of state. Appendix A shows the numerical results for the same case study using a simplified thermodynamic model.

3.2 Difference between design and operation

There are fundamental differences between optimal design and optimal operation. In the first case we need to find the equipment that minimizes the total cost of the plant (investments and operational costs). In the latter case however, the equipment is given so we only need to consider the operational costs.

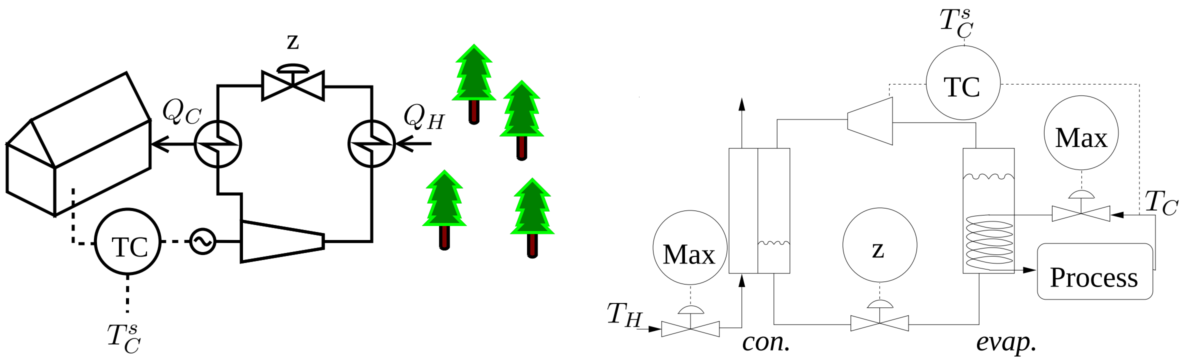


Figure 5: Cold warehouse with ammonia refrigeration unit

A typical approach when designing heat exchanger systems is to specify the minimum temperature differences (pinch temperatures) in the heat exchangers (see Equation 2). In operation this is no longer a constraint, but we are given a certain heat transfer area by the design (see Equation 3).

$$\begin{aligned} \min \quad & Ws \\ \text{such that} \quad & T_C - T_C^s = 0 \\ & \Delta T - \Delta T_{\min} \geq 0 \end{aligned} \tag{2}$$

$$\begin{aligned} \min \quad & Ws \\ \text{such that} \quad & T_C - T_C^s = 0 \\ & A_{\max} - A \geq 0 \end{aligned} \tag{3}$$

The two optimization problems are different in one constraint, so there might be a different solution even with the same conditions.

We will now solve the two optimization problems in Equation 2 and 3 with the following conditions:

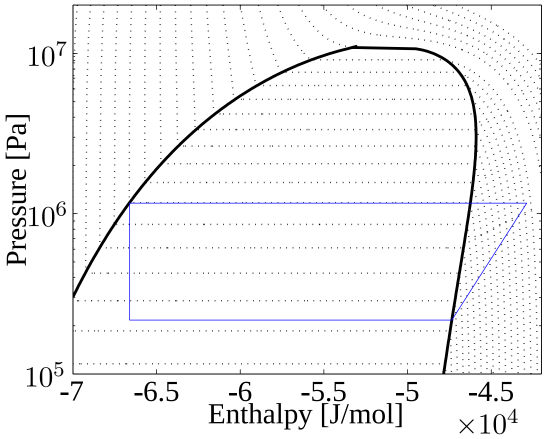
- Ambient temperature T_H = 25 $°C$
- Indoor temperature set point T_C^s = -12 $°C$

Temperature control maintains $T_C = T_C^s$ which indirectly gives $Q_C = Q_{loss} = UA \cdot (T_H - T_C)$. The minimum temperature difference in the heat exchangers are set to ΔT_{min} =5 $°C$ in design. In operation the heat exchanger area A_{max} is fixed at the optimal design value.

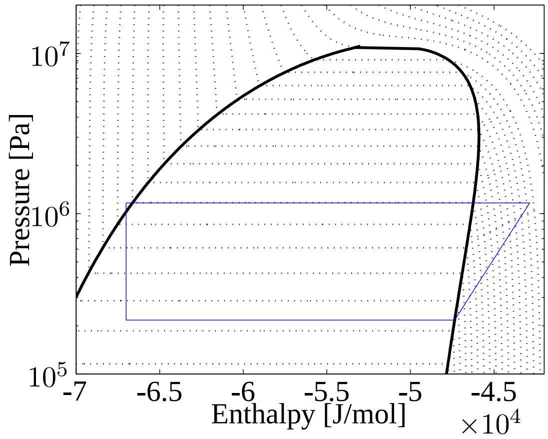
Figure 6(a) shows pressure enthalpy diagram for the optimal design with no sub-cooling in the condenser. In operation however, there is sub-cooling as seen in Figure 6(b).

Conclusion: For this ammonia cycle, sub-cooling by 4.66 $°C$ reduces the compression work W_s by 1.74% which is contrary to popular belief. The high pressure P_{con} is increases by 0.45%, but this is more than compensated by a 2.12% reduction in flowrate. The condenser charge M_{con} is increased by 5.01% in optimal operation.

Similar results are obtained for a CO_2 cycle using Span-Wagner equation of state (Span and Wagner, 1996).



(a) Optimal design



(b) Optimal operation

Figure 6: Difference in optimal design and optimal operation for same conditions

Table 3: Difference between optimal design and optimal operation

	W_s $[W]$	Flow $[mol/s]$	M_{con}[a] $[mol]$	ΔT_{sub} $[K]$	P_{con} $[Pa]$	P_{evap} $[Pa]$	A_{con} $[m^2]$	A_{vap} $[m^2]$
Design	4648	1.039	17721	0.00	1162860	216909	8.70	4.00
Operation	4567	1.017	18609	4.66	1168120	216909	8.70	4.00

[a] Evaporator charge has no effect

3.3 Implementing optimal operation

From section 2 we will have one unconstrained degree of freedom left to optimize the operation. In this section we are evaluating what should be controlled with this remaining degree of freedom. First we use a linear model to obtain promising candidate controlled variables. The most promising control structures are then evaluated on the non-linear model to identify possible infeasibility problems or non-linearities leading to poor performance far from nominal operating point.

The heat exchanger areas from the analysis above is utilized also in this section, but we assume that the process is slightly over-designed (to be able to operate at poorer conditions than nominally). Conditions:

- Condenser area: 8.70 m^2
- Evaporator area: 4.00 m^2
- T_H=20$°C$
- T_C^s=-10$°C$
- UA=500W/K

3.3.1 Linear analysis of alternative controlled variables (CV's)

To find promising controlled variables the method in (Skogestad, 2000) will be utilized. In short:
We are looking for variables which optimal value (y_{opt}) change little when the system is exposed to disturbances. We also need a sufficient gain from the input to the variable ($G = \frac{\Delta y}{\Delta u}$).
Procedure:

- Make a small perturbation in all disturbances (same fraction of expected disturbance) and re-optimize the operation to find the optimal change in each variable for each disturbance ($\Delta y_{opt}(d_i)$). Large $\Delta y_{opt}(d_i)$ indicates control problems for disturbance i.
- Do a perturbation in the independent variables (u) to find the gain ($G = \frac{\Delta y}{\Delta u}$).
- Scale with respect to inputs such that all the inputs have equal effect on the objective function (not necessary in this case since there is only one manipulated input)
- Scale the gain with $span\ y = \sqrt{\sum_i \Delta y_{opt}(d_i)^2}$ and implementation error n: $G' = \frac{G}{span\ y + n}$

We are looking for variables with large scaled gains G'.

In this case study we only have one independent variable $u = z$ (choke valve opening). The following disturbance perturbations are considered (1 % of expected disturbance):

$\hat{d}_1$: $\Delta T_H = \pm 0.1\ °C$

$\hat{d}_2$: $\Delta T_C^s = \pm 0.05\ °C$

$\hat{d}_3$: $\Delta UA = \pm 1\ W/K$

The heat loss is given by Equation 4, and temperature control will indirectly give $Q_C = Q_{loss}$.

$$Q_{loss} = UA \cdot (T_H - T_C) \tag{4}$$

Table 4: Linear analysis of the ammonia case study

Variable		G	span y	n	G'
Con. pressure P_h	[Pa]	-1.33e6	9142	1.0e5	12.2
Evap. pressure P_l	[Pa]	0.00	1088	3.0e4	0.00
Valve opening z	[-]	1	0.0019	0.01	84.0
Liq. level in evap.	$[m^3]$	7.48	0.0083	0.01	410
Liq. level in con.	$[m^3]$	-8.21	0.0094	0.01	424
Temp. out of con.	[K]	274	0.3120	1.00	209
ΔT_{sub}	[K]	-318	0.4663	1.50	162
ΔT at con. exit	[K]	-274	0.4026	1.50	144

Table 4 shows the linear analysis presented above. Some notes about the table:

- This is a linear approach, so for larger disturbances we need to check the promising candidates for nonlinear effects.

- The procedure correctly reflects that pressure control is bad, being infeasible (evaporator pressure) or far from optimal (condenser pressure).

- The loss is proportional to the inverse of squared scaled gain ($Loss = (1/G')^2$). This implies that a constant condenser pressure would result in a loss that is 47 times larger than a constant valve opening.

- Liquid level in evaporator is a common way to control flooded evaporator systems (Langley, 2002), there are however other candidates that also are promising. Liquid level in condenser (also a scheme showed in (Langley, 2002)) is best according to the linear analysis.

- Controlling the temperature out of the condenser looks promising (we will later see that this is not working on the non-linear model)

- Controlling the degree of sub-cooling in the condenser is slightly better than controlling the temperature difference at condenser outlet

3.3.2 Nonlinear analysis of promising CV's

The nonlinear model is subjected to full disturbances (shown below) and for each control policy we have included the implementation error n from Table 8.

d_1: $\Delta T_H = +10°C$

d_2: $\Delta T_H = -10°C$

d_3: $\Delta T_C^s = +5°C$

d_4: $\Delta T_C^s = -5°C$

d_5: $\Delta UA = +100\ J/K$

d_6: $\Delta UA = -100\ J/K$

As predicted from the linear analysis controlling P_h or z should be avoided as it results in infeasibility or poor performance. Although controlling condenser outlet temperature seems like a good strategy from the linear analysis it proves poor far from nominal operating point, and results in infeasible operation. Controlling the degree of sub-cooling ΔT_{sub} gives small losses for some disturbances, but results is infeasible for others. So we are left we three candidates and the worst case loss for each are as follows:

1. Liquid level in condenser: V_l^{con}: 0.19 %

2. Liquid level in evaporator V_l^{vap}: 0.45 %

3. Temperature difference at condenser outlet ΔT^{out}_{con}: 1.49 %

Remark. Control of both condenser and evaporator liquid level are used in heat pump systems (Langley, 2002)

Remark. According to (Larsen et al., 2003) a constant condenser pressure is most frequently used in refrigeration systems, but according to the results above this will give large losses and infeasible operation.

Remark. Another good policy is to maintain constant temperature difference out of the condenser. This control policy has as far as we know not been reported in the literature, but has been considered used in CO_2 heat pumps.

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A Ammonia case study with simplified thermodynamic model

In this section the ammonia case presented in section 3 is studied with a simplified thermodynamic model. Mostly results are shown here, so the reader is advised to consult the corresponding sections in chapter 3. This section is used as an example in (Skogestad and Postlethwaite, 2005) on page 398.

A.1 Thermodynamic model

The heat capacities are assumed constant in each phase. Liquid phase is assumed incompressible and gas phase is modeled as ideal gas. Vapour and liquid enthalpy are given by Equation 5 and 6 respectively.

$$h_v(T) = c_{P,v} \cdot (T - T_{ref}) + \Delta_{vap}h(T_{ref}) \tag{5}$$

$$h_l(T) = c_{P,l} \cdot (T - T_{ref}) \tag{6}$$

Thermodynamic data are collected from (Haar and Gallagher, 1978) using T=267.79K as reference temperature. Table 5 summarize the used quantities.

$c_{P,l}$	77.92	$J/(mol\ K)$
$c_{P,v}$	43.81	$J/(mol\ K)$
$\Delta_{vap}h(T_{ref})$	21.77	$kJ/(mol\ K)$
ρ_l	37.99	$kmol/m^3$

Table 5: Thermodynamic data

Saturation pressure is calculated from Equation 7 (Haar and Gallagher, 1978) with parameters given in Table 6. P_c and T_c are critical pressure and temperature respectively. $\omega = T/T_c$.

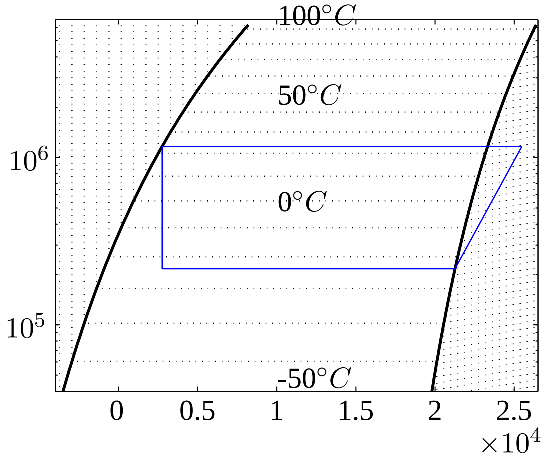
$$log_e(P/P_c) = 1/\omega \left[A_1(1-\omega) + A_2(1-\omega)^{3/2} + A_3(1-\omega)^{5/2} + A_4(1-\omega)^5\right] \tag{7}$$

A_1 =	-7.296510	T_c = 405.4	K
A_2 =	1.618053	P_c = 111.85	bar
A_3 =	-1.956546		
A_4 =	-2.114118		

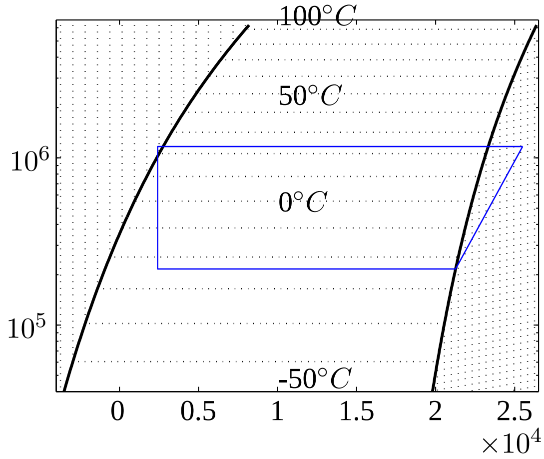
Table 6: Parameters used to calculate saturation pressure

A.2 Difference between design and operation

- T_H = 25$°C$
- T_C = -12$°C$
- UA = 540 J/K



(a) Optimal design



(b) Optimal operation

Figure 7: Difference in optimal design and optimal operation for same conditions

Table 7: Difference between optimal design and optimal operation

	W_s $[W]$	Flow $[mol/s]$	M_{con}[a] $[mol]$	ΔT_{sub} $[K]$	P_{con} $[Pa]$	P_{evap} $[Pa]$	A_{con} $[m^2]$	A_{vap} $[m^2]$
Design	4565	1.08	9330	0	1166545	216712	6.55	4.00
Operation	4492	1.06	9695	4.48	1170251	216712	6.55	4.00

[a]Evaporator charge has no effect

A.3 Linear analysis of alternative controlled variables (CV's)

- T_H = 20°C
- T_C = -10°C
- UA = 667 J/K

$\hat{d}_1$: ΔT_H=+0.1 °C

$\hat{d}_2$: ΔT_C^s=+0.05 °C

A.4 Nonlinear analysis of promising CV's

- T_H = 20°C
- T_C = -10°C
- UA = 667 J/K

Table 8: Linear analysis of the ammonia case study

Variable		$\Delta y_{opt}(\hat{d}_1)$	$\Delta y_{opt}(\hat{d}_2)$	G	$\lvert G'(\hat{d}_1)\rvert$	$\lvert G'(\hat{d}_2)\rvert$
P_h	[Pa]	3689	3393	-464566	126	137
P_l	[Pa]	-167	418	0	0	0
T_{out}^{con}	[K]	0.1027	0.1013	316	3074	3115
ΔT_{sub}	[K]	0.0165	0.0083	331	20017	39794
z	[-]	8.00E-4	3.00E-5	1	1250	33333
V_l^{con}	[m^3]	6.7E-6	4.3E-6	-1.06	157583	244624
V_l^{vap}	[m^3]	-1.00E-5	-1.00E-5	1.05	105087	105087

The nonlinear model is subjected to full disturbances:

d_1: $\Delta T_H = +10°C$

d_2: $\Delta T_H = -10°C$

d_3: $\Delta T_C^s = +5°C$

d_4: $\Delta T_C^s = -5°C$

Table 9 shows the loss compared with re-optimized operation for different control policies.

Table 9: Loss for different control policies

	ΔW_s [%]			
Constant	d_1	d_2	d_3	d_4
Valve opening z	10.8	12.0	9.8	12.7
Con. pressure P_h	Inf	43	2.5	Inf
Temp. out of con.	Inf	Inf	0.0079	0.0086
Liq. level evap.	0.013	0.012	$1.34 \cdot 10^{-5}$	0.00
Liq. level con.	0.0024	0.003	$4.2 \cdot 10^{-4}$	$2.8 \cdot 10^{-4}$
Sub-cooling ΔT_{sub}	0.39	4.0	0.69	0.131

Inf = Infeasible

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