



DIPLOMA WORK 2007

Title: Optimal operation of cooling cycle/LNG process	Subject (3-4 words): Vapour compression cycles, LNG, optimization, degrees of freedom, control structures
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ABSTRACT <p>Goal of work (key words): The goals of the diploma work has been to study the dynamic operation of cooling processes using a commercial simulation software (Aspen HYSYS). The processes treated in this work are a simple ammonia cooling cycle and the C3-MR process for liquefaction of natural gas (LNG). Goals for ammonia cycle: To see if results from earlier work could be validated using Aspen HYSYS and simulating the cycle dynamically, study optimization of the process and to test different control setups for the cycle. Goals for LNG process: To identify degrees of freedom available for control and optimization, propose a control structure based on this, build a dynamic model and, if sufficient time, use the dynamic model to test the proposed control structure in dynamic simulations.</p> <p>Conclusions and recommendations (key words):</p> <p>For the ammonia cycle, it was found that subcooling at condenser outlet was optimal, as stated by earlier studies. This subcooling was also found to be a good candidate for controlled variable in the process, along with the condenser outlet temperature difference.</p> <p>For the C3-MR process, it was found that one degree of freedom is available for process optimization. A dynamic model has been built and a control structure has been proposed. Further work on this process could include improving the dynamic model and doing optimization and control studies on the process.</p>	
<p>I declare that this is an independent work according to the exam regulations of the Norwegian University of Science and Technology</p> <p>Date and signature:</p>	

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1 Introduction

This thesis is taking up the thread from work done at Norsk Hydro's Oil and Energy Research Centre in Porsgrunn in the summer of 2006, and the subsequent specialisation project in Process Systems Engineering at NTNU in the autumn of 2006. The study project at Norsk Hydro in 2006 dealt with steady-state modelling of the Air Products C3-MR process for liquefaction of natural gas, and the specialization project dealt with dynamic modelling and simulation of the propane precooling section of the C3-MR process. In this diploma work, the focus is moved from the process modelling itself to using process models to study operation of cooling cycles. In other words, the focus is on process control, and to some extent optimization, rather than on process modelling.

The main goals of this diploma project are to study dynamic operation and control of a cooling cycle using a commercial simulation software (Aspen HYSYS 2004.2 is used), to propose a good control structure for a complex LNG process, to model the system dynamically and, if there is sufficient time, to test the proposed control structure.

Previous work on the ammonia cycle by Jørgen B. Jensen and Sigurd Skogestad [1] covers steady-state operation and optimization, but has not studied dynamics and control. Therefore some of the focus on the ammonia cycle in this diploma work has been to validate conclusions from [1] in dynamic simulations.

2 Background

2.1 Process control

The focus of this project has been operation and control of cooling cycles, so process control should get some emphasis. There are some topics that need to be described:

- Degree of freedom analysis. An understanding of the degrees of freedom in the process is necessary to realize which and how many variables are available for optimization of the operation.
- Self-optimizing control. This is important when one wants to choose what variables to control with the available degrees of freedom. One wants to choose variables that are suited to maintain optimal operation without needing to re-optimize when disturbances occur.
- Tuning of controllers. When one has chosen the controlled variables and pairing of controlled and manipulated variables, the individual controllers need to be tuned in order to assure that the controllers do what we want them to.

2.1.1 Degrees of freedom from the perspectives of process optimization and control

Generally speaking, an equation system's number of degrees of freedom (DOF) is defined as the number of variables minus the number of independent equations (meaning the number of additional variable specifications needed for the system to be solved). When dealing with process control, the degrees of freedom takes a slightly different meaning; the degrees of freedom available for process control is the number of variables that can be manipulated. These include valve positions, compressor speeds, and other adjustable objects.

When dealing with optimization, there will be less DOFs. This is because there are typically several variables that must be controlled, but do not have any effect on the steady state. The most important example is any holdups (tanks etc.) in the process. Each controlled level consumes one DOF. There may also be that some of the manipulated variables do not have any steady state effect.

Generally there are some specifications that the process should accomplish, and some variables that are not allowed to be outside a certain range. This means some of the manipulated variables will be needed to control process specifications and constraints.

The number of DOFs available for optimization are then the number of manipulated variables minus the sum of controlled holdups, MVs with no

steady state effect, active constraints and specifications. The procedure of identifying the degrees of freedom is described by Skogestad ([2]).

2.1.2 Self-optimizing control

When the degrees of freedom are known, it must be decided which process variables they should be used to control. If there are unstable variables like the temperature in an exothermic reactor (especially if the conversion is low and potentially can increase a lot) these must be controlled. But one may still have one or more manipulated variables left. When deciding what to use these for, the idea of self-optimizing control comes into the discussion.

When a process is running at its optimum conditions and disturbances are introduced, the optimal values of the unconstrained variables will change. (The active constraints may also change, this is not considered here). If one controls these variables at a constant value rather than reoptimizing, the objective function for the optimization of the process will have a higher value than it could have. The difference is regarded as loss. *The self-optimizing variables are the variables which, when kept constant, makes this loss as small as possible.* According to Skogestad [2], the variables should meet these requirements:

- The optimal value of the controlled variable (CV) should be insensitive to disturbances
- The CV should be easy to measure and control (i. e. a small implementation error)
- The CV should be sensitive to changes in the manipulated variables (MV) and the optimum (the minimum of the cost function as function of the CV) should be flat
- If there are more unconstrained degrees of freedom, one should select independent controlled variables

2.1.3 Pairing of variables, tuning of PID controllers

When the controlled variables have been chosen, one must decide which manipulated variable (MV) should be linked with which controlled variable (CV). One should pair variables in such a way that the MV has a large effect on the CV, and any time lag from a change in the MV to response in CV should be short. The latter argument means that the variables should, physically, be located close to each other, unless the response is transferred quickly through the process (the latter is, for example, the case for pressures).

The final step in setting up the basic control structure is to decide the controller parameters - gain, integral time and derivative time. This can

be done in several ways - by pure trial and error, or using some kind of tuning rules. These include Ziegler-Nichols, IMC and other (different tuning methods are described in [3]). Here, the SIMC rules (Skogestad, [4]) have been used.

When using the SIMC rules, one needs a transfer function - typically of first order with delay (transfer function $g(s) = k \frac{e^{\theta s}}{\tau s + 1}$), or integrating ($g(s) = k \frac{e^{\theta s}}{s}$). The transfer functions may be taken from a theoretical process model or from process measurements. For a theoretical approach, one may have transfer functions of higher order than one, these can be approximated to a first order process using the so-called *half rule*, also described in [4]. For the empirical approach, the procedure is to perform a step in the manipulated variable and measure the controlled variable's open-loop response, and then finding a first-order or integrating approximation to this response.

The SIMC rules for tuning of controllers (for first-order and integrating processes) are shown in table 1. K_c and τ_I are the controller parameters (for PID control, the derivative time τ_D would also be required), and these are expressed as function of the transfer function parameters and the tuning parameter τ_c . τ_c should be small for quick control and large for robust control. The SIMC rules propose $\tau_c = \theta$.

Table 1: SIMC tuning rules for first-order and integrating processes

Process	K_c	τ_I
First-order	$\frac{1}{k} \frac{\tau_1}{\tau_c + \theta}$	$\min[\tau_1, 4(\tau_c + \theta)]$
Integrating	$\frac{1}{k} \frac{1}{\tau_c + \theta}$	$4(\tau_c + \theta)$

2.2 About vapour compression cycles

Simple vapour compression cycles are the most common processes used for refrigeration when the desired temperature is lower than the temperature of available cold utilities like cold water. They are used in refrigerators, cold stores, and in air conditioning. The principle is to remove heat from the 'system' at a low temperature T_c , and delivering the heat to the surroundings at a temperature T_h , by adding work, in form of a compressor doing a shaft work W_s on the refrigerant. A general vapour compression cycle consists of four steps:

- The refrigerant is compressed to a high pressure, bringing its temperature above the temperature of the cold utility (often air or water). Temperature is now T_1 , pressure is P_h .
- The refrigerant is condensed by the cold utility, it is now liquid at T_2 , P_h .

- The liquid refrigerant is flashed across a valve, bringing it to a temperature T_3 and a pressure P_l . The temperature T_3 is lower than the temperature at which cooling is to be provided (T_c).
- The liquid refrigerant is vaporized, removing heat from the system that is to be cooled. It leaves the vaporizer at T_4 , P_l .

A flow sheet of a general vapour compression cycle is shown in figure 1. Figure 2 shows a typical pressure-enthalpy diagram for a vapour compression cycle. This diagram is taken from [5].

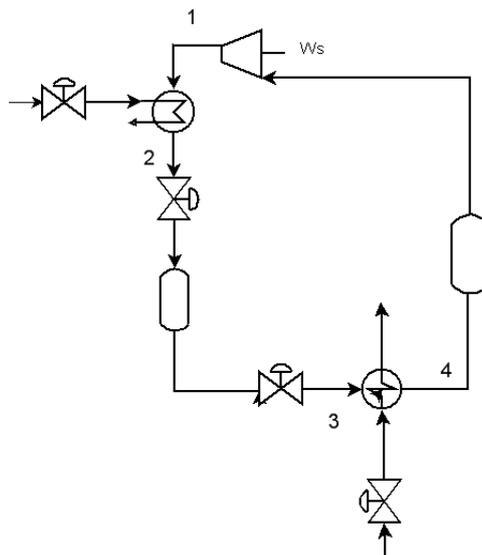


Figure 1: Flowsheet of vapour compression cycle

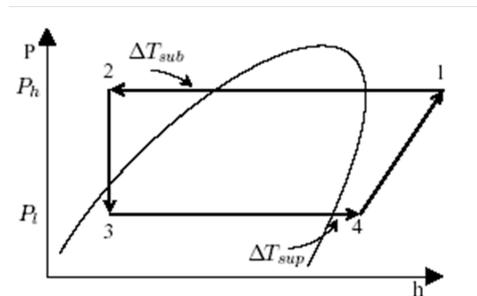


Figure 2: Pressure-enthalpy diagram of vapour compression cycle

The required shaft work depends on the temperatures T_c and T_h . The larger the difference, the larger the required work. One can define the co-

efficient of performance (COP) of a cooling cycle as $COP = \frac{Q_c}{W_s}$ where Q_c is the amount of heat removed from the ‘system’. The theoretical limit for the COP is the Carnot efficiency COP_{Carnot} , which for a cooling cycle is defined as

$$COP_{Carnot} = \frac{T_c}{T_h - T_c} \quad (1)$$

The Carnot efficiency will never be achieved in a real process, as it is based on an ideal process where all steps are reversible. This is not possible in a real process. Although the valve may be replaced with a turbine, thus retrieving some work from the expansion, one will always have friction loss in the process equipment. And even if a turbine is used, there will be some heat loss leading to non-adiabatic compression and expansion. One can define the cycle’s efficiency as

$$\mu = \frac{COP_{real}}{COP_{Carnot}} \quad (2)$$

The value of μ will always be smaller than 1.

2.3 Liquefaction of natural gas

When transporting natural gas over long distances, it is common to transport it in the form of liquefied natural gas, LNG. The process of liquefying the gas is usually done on-shore, and the LNG plant itself may or may not be integrated with other gas treatment plants and petrochemical plants.

In a typical LNG process, the refrigerant is usually cooled in the same exchanger as the natural gas; high-pressure refrigerant is first condensed, completely or partially, with sea water (or less frequently, air) before it is sent through the main heat exchanger, where it leaves at approximately the same temperature as the natural gas. It is flashed to obtain lower temperature, and then it is used to cool both itself and the natural gas. It is then compressed and condensed again. An example of the simplest kind of LNG process is the PRICO process ([6]).

In other, more complex processes, the refrigerant and the natural gas are both cooled with another, secondary refrigeration cycle. In the C3-MR process ([7]), both the natural gas and the refrigerant (labeled MR, mixed refrigerant) are cooled with propane to below -30°C before entering the main exchanger. The composition of the mixed refrigerant may be adjusted to match the cooling requirements.

There are also processes where the refrigerant in the pre-cooling cycle is cooled by another refrigerant in an additional cooling cycle. Processes of this kind are called cascade processes. The refrigerants in each cycle may be pure fluids or mixtures. An example of a cascade process is the Statoil-Linde mixed-fluid cascade (MFC) process [8].

In LNG processes, the ultimate limit to the production rate is the maximum available compressor power. If there are other units in the process that limit production, one will try to remove those constraints in order to utilize the compressor power better. When optimizing LNG plant operation, one seeks to maximize the LNG production rate for a given compressor power consumption. Different pressure settings and different compositions of mixed refrigerants are among the variables that are adjusted to give optimal operation.

2.4 Modelling and simulation in HYSYS

When simulating cooling processes, one must model compressors, heat exchangers and valves.

Compressors can be modelled with a specified, constant efficiency, or the user can supply compressor curves where the efficiency is calculated as a function of volumetric flow for different compressor speeds. If the efficiency is set, compressor speed is not taken into the calculations, and the manipulated variable of the compressor is the shaft work W_s . It is also possible to supply surge curves, if one is to simulate compressors with surge control. But for simple studies, using constant efficiency is often sufficient.

Heat exchangers have several calculation models that can be used. In steady state mode, there are end-point and weighted design models as well as steady state rating. For dynamic rating, two models are available; a basic model and a detailed model.

The basic model is based on an end-point calculation using the standard heat transfer equation(3). One specifies the value of the product UA , and also the k value in the pressure-flow equation (4). HYSYS can also calculate this k value if the nominal flow and pressure drop are given.

$$Q = UA\Delta T_{lm}f_t \quad (3)$$

$$f = \sqrt{\rho} \cdot k \cdot \sqrt{\Delta P} \quad (4)$$

The detailed model divides the exchanger into zones and solves the heat transfer equation for each zone individually. When using the detailed model, the user must specify all relevant geometric data; shell and tube dimensions, baffle cut, spacing and orientation of the baffles, shell and head TEMA type, number of tube passes. The heat transfer coefficients and pressure drops may be calculated from the specified geometric data and feed streams, or they can be specified (for the case of pressure drops, the k value will be the specification used in dynamic simulation).

For the valves, there are three different sizing methods; these are the C_V , C_g and k methods. For the k method, the pressure drop and flow are linked through an equation similar to equation 4, with the valve opening Z in %

multiplied in on the right hand side. For a description of the other methods and their corresponding equations, see the HYSYS Operations Guide ([9]).

A more detailed description of the heat exchanger model can also be found in [9].

3 Case study: Simple ammonia cycle

In order to build a better understanding of operation of cooling cycles, a simple ammonia cycle was studied. The considerations about degrees of freedom, and the significance of different process configurations, applies to simple cycles just as it does for complex processes like the C3-MR process.

An optimization was carried out to validate the conclusion in a study done by Jensen and Skogestad [1], which states that some subcooling at the condenser outlet gives optimal operation. The other parts of this case study were:

- Degree of freedom analysis of the model
- Choosing the controlled variables
- Tuning the controllers
- Testing the control setup by introducing different disturbances

3.1 Process description

The cycle considered here is a simple cycle (see figure 3) with a compressor, a condenser, a vaporizer and liquid tanks after the condenser and vaporizer. The first, as well as the extra valve on the high-pressure side of it, was necessary to allow for controlled subcooling at the condenser outlet, the latter being needed to avoid liquid being fed to the compressor. (At steady state, the liquid entering the high-pressure tank would be saturated, i. e. no subcooling, meaning the valve between the condenser and the receiver would define the subcooling).

3.2 Modelling the cycle

When building the steady state model of the cycle, it was attempted to keep the process conditions close to the ones used in [1], to make comparison easy.

The SRK (Soave-Redlich-Kwong) fluid package was used for thermodynamical calculations in the model. The compressor was modelled with constant efficiency, meaning the shaft work W_s was the variable that could be manipulated, rather than speed.

For heat exchanger rating the basic model was used for the vaporizer. For the condenser, the detailed model was used. All valves were sized using the C_V method.

It should be noted that in [1], the temperatures T_c and T_h are assumed constant. This is reasonable for cross-flow exchangers (in cooling processes, this type of exchangers is common). When modelling a shell and tube heat exchanger in HYSYS, this can not be fully achieved. However, using a large mass flow or a vaporizing/condensing fluid will assure the temperatures are

close to constant. As long as the temperature change is small compared to the mean temperature difference in the exchanger, the results will probably not be influenced much.

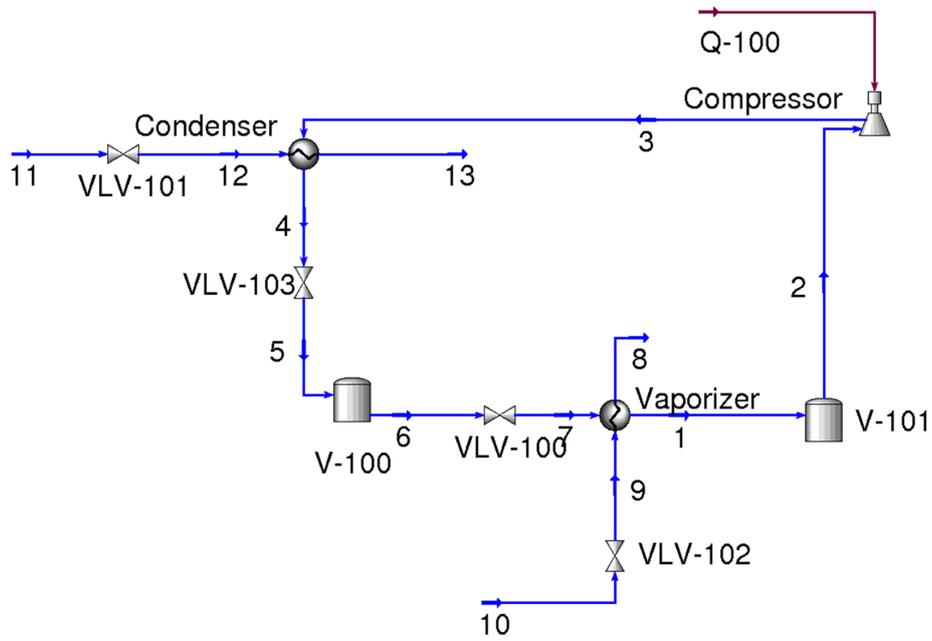


Figure 3: HYSYS flowsheet of NH₃ cycle

The different model data are shown in tables 2, 3 and 4. The temperatures and pressures in table 4 refer to figures 1 and 2.

Table 2: Initial steady state values of stream data

Variable	Value
T_c	$-10\text{ }^\circ\text{C}$
T_h	$20\text{ }^\circ\text{C}$
P_h	1070 kPa
P_l	235 kPa
F	0.743 mol/s
T_1	102.8 $^\circ\text{C}$
T_2	20.5 $^\circ\text{C}$
T_3	$-14.5\text{ }^\circ\text{C}$
T_4	$-14.6\text{ }^\circ\text{C}$
Condenser water flow	1500 kmol/h
Vaporizer air flow	2040 kmol/h
Condenser duty	16.47 kW
Vaporizer duty (Q_c)	15 kW
Compressor shaft work	2,963 kW

Table 3: Process parameter specifications

Parameter	Value
Condenser UA	1273 W/K
Vaporizer UA	3764 W/K
Compressor efficiency	0.95
VLV-103 ΔP	188 kPa
VLV-100 ΔP	636 kPa
Tube side ΔP in condenser	10 kPa
Shell side ΔP in condenser	5 kPa
Tube side ΔP in vaporizer	10 kPa
Shell side ΔP in vaporizer	1.0 kPa
Vaporizer shell volume	0.2 m ³
Vaporizer tube volume	0.2 m ³
Volume of V-100	0.2 m ³
Volume of V-101	2 m ³

Table 4: Geometric and other data for condenser

Parameter	Value
Shell passes	1
Tube passes	2
TEMA type	AEU
Shell diameter	800 mm
Tubes per shell	280
Tube pitch	50 mm
Tube layout angle	30°
Baffle cut	20 %
Baffle spacing	800 mm
Tube inner/outer diameter	20 mm/16 mm
Tube length	2 850 mm
Shell HT coefficient	500 $\frac{kJ}{h \cdot m^2 \cdot K}$
Tube HT coefficient	500 $\frac{kJ}{h \cdot m^2 \cdot K}$
Zones per shell pass	10

3.3 Degrees of freedom analysis

The flow sheet in figure 3, which illustrates the HYSYS model of the cycle, shows that the process has five variables that can be manipulated. These are the four valves, and the compressor shaft work W_s (illustrated by the energy stream Q-100 in the flow sheet). The two valves V-101 and V-102 keep the mass flow in streams 10 and 11 in the flow sheet constant. There are three manipulated variables left. As there are two tanks in the cycle, the holdup in one of these must be controlled (discussed in [5]). This consumes one manipulated variable. The cooling load (Q_c) delivered by the cycle also needs to be controlled, meaning there is one unconstrained degree of freedom left. *This degree of freedom can be used to optimize the operation of the cycle.*

3.4 Selection of controlled variables

As mentioned above, the valves V-101 and V-102 control the mass flows in streams 10 and 11 at constant values. The three remaining manipulated variables should control one liquid level, the cooling duty Q_c and a third variable that should, ideally, be a self-optimizing variable.

In this case study it was decided to use the compressor work W_s to control the cooling duty, and to use VLV-100 to control the level of V-100, leaving the level of V-101 uncontrolled. Then the valve VLV-103 was available for controlling a variable that could be chosen among the unconstrained variables in the process. According to [1], the temperature difference at the condenser outlet ($\Delta T = T_2 - T_h$) is a good variable to control, as it gives small loss and its sensitivity to implementation error is small. Other variables that are mentioned as good candidates are the degree of subcooling at the condenser outlet ($\Delta T_{sub} = T_{sat,Ph} - T_2$) and the liquid levels in the condenser and the liquid receiver after the condenser¹ (equivalent to controlling the level in a flooded vaporizer). Control of some variables are infeasible if the disturbances are large, these variables include the condenser exit temperature T_2 and the compressor outlet pressure P_h .

The variables that were tested in this study were the condenser outlet ΔT , the ΔT_{sub} and P_h (the last being tested to see if it would give satisfying control in the feasible region). Figure 4 shows the HYSYS flow sheet with controllers.

3.5 Optimization, optimality of subcooling

The study done by Jensen and Skogestad [1] stated that some sub-cooling of ammonia at the condenser outlet would give optimal operation (i. e. minimal power consumption). To check if this could be validated in a dynamic

¹The paper considers a cycle with only one liquid receiver, and the level in the receiver is not necessarily controlled. For the cycle with two receivers, this control scheme would correspond to controlling either the level in V-101 or the level in the condenser

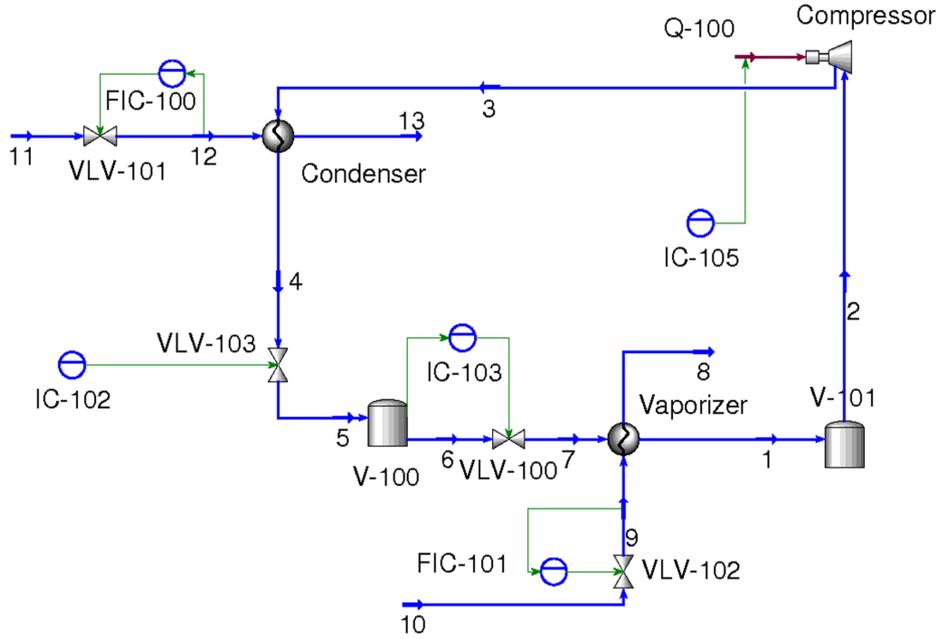


Figure 4: Flowsheet of NH_3 cycle with controllers shown

simulation, the ‘optimization DOF’, i. e. the position of valve V-103 in the flow sheets, was changed in steps to see if an optimal position could be found. If subcooling was optimal, this would mean the optimal position of the valve would be less than 100 % open (a 100 % open valve means the condition of the NH_3 does hardly change at all from the condenser outlet to the inlet of V-100, and since the outlet stream of this tank is saturated liquid, the condenser outlet stream will also be saturated at steady state, hence no subcooling). If the optimization should show that it was optimal to leave VLV-103 fully open, it would imply that the design with a high-pressure liquid receiver and an extra valve was sub-optimal.

The level controller (IC-103 in figure 4) and the Q_c controller (IC-105) were tuned roughly, by trial and error. The parameters are shown in table 5.

Table 5: Settings of level and load controllers for optimization study

Controller	K_c	τ_I (minutes)
IC-103	0.5	18
IC-105	0.5	20

With the level and load controllers tuned, the opening (z) of VLV-103 was changed from 75 % to 97,5 % in 2,5 % steps. Between each step, the

process was given 100 minutes to stabilize. Figure 5 shows the stepping in valve position from 75 to 97.50 % and the response in compressor power. Table 6 summarizes some of the important variables.

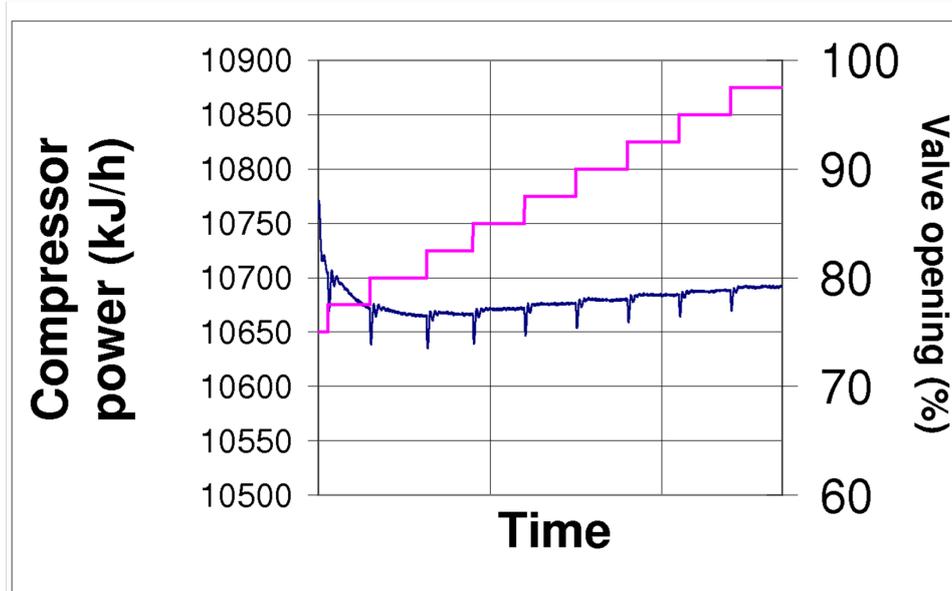


Figure 5: Response in compressor power to stepping in opening of VLV-103

Table 6: Results of stepping the valve position (Z)

Z (%)	ΔT_{sub} ($^{\circ}\text{C}$)	F (kmol/s)	W_s (kJ/h)	P_h (kPa)
77,5	2,59	2,711	10673	1047,0
80,0	2,42	2,710	10665	1046,6
82,5	2,28	2,711	10666	1046,5
85,0	2,14	2,713	10671	1046,4
87,5	2,02	2,714	10676	1046,3
90,0	1,92	2,716	10680	1046,2
92,5	1,81	2,716	10684	1046,2
95,0	1,72	2,717	10688	1046,1
97,5	1,63	2,719	10691	1046,1

Figure 5 and table 6 indicate that there is an optimum when the valve VLV-103 is approximately 80 % open. At this point and with the model parameters used here, the subcooling is approximately 2,50 $^{\circ}\text{C}$. However, the optimum is very flat, meaning that the saving in compressor power between a 80 % open valve and a 100% open valve is not very large.

3.6 Control setup

3.6.1 Pairing of manipulated and controlled variables

As described in section 3.4, valves VLV-101 and VLV-102 were set to keep constant flow rates in streams 10 and 11. The compressor shaft work (W_s) was used to control the cooling duty (Q_c), and the choke valve (VLV-100) was used to control the holdup in V-100 (the high pressure liquid receiver).

The last manipulated variable (opening, z , of VLV-103) was used for control of three different variables, of which the first two were recommended as good choices by [1]:

- The temperature difference in the cold end of the condenser (ΔT)
- The degree of subcooling at the condenser outlet (ΔT_{sub})
- The pressure at the condenser inlet (P_h)

3.6.2 Tuning of controllers

The tuning of the controllers was performed by using step responses to find approximate transfer functions.

Figure 6 shows the response in cooling duty (or load) to a step increase in compressor power from 35 to 40 %.

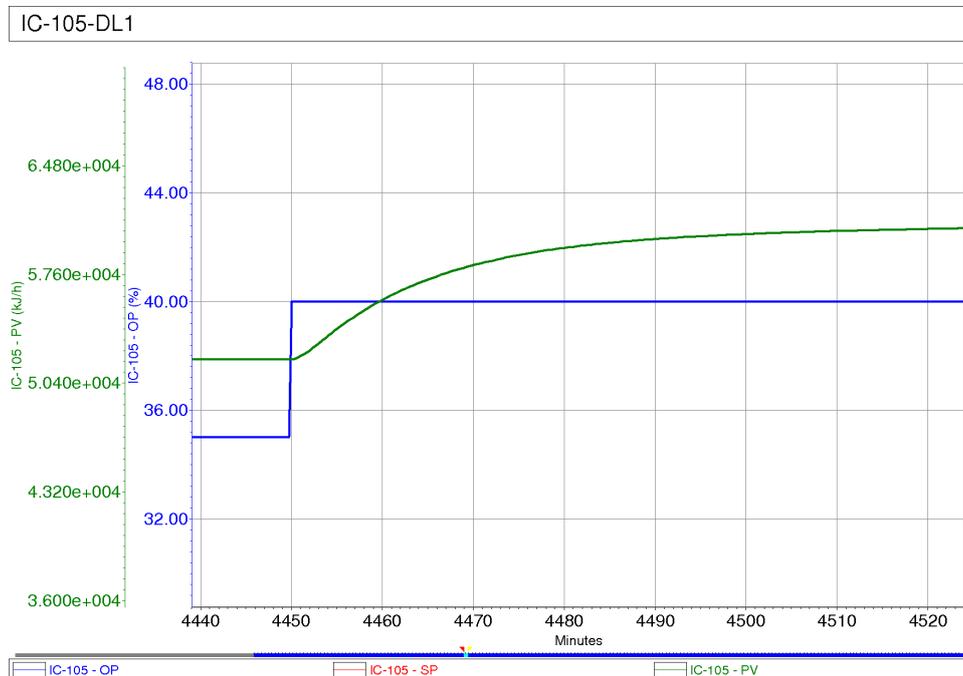


Figure 6: Response in Q_c to a step in W_s

To find the steady-state gain (k in the first-order transfer function), one must first find the change in the measured variable (PV in HYSYS controllers) in % of the range that is defined for the controller (by the user). For this controller, the range for process variable was defined to be from 0 to 108 000 kJ/h, so the percentwise change becomes

$$\Delta Q_c = \frac{60700 - 52000}{108000} \cdot 100\% = 8,06\%$$

To find the gain from input to output, one must divide by the step size (in % of the maximal) in the manipulated (input) variable:

$$k = \frac{\Delta Q_c}{\Delta W_s} = \frac{8,06\%}{5\%} = 1,61$$

To find the time constant τ , one uses that after τ minutes, approximately 63,2 % of the change in the output variable is done. That is, one must read from the graph the time when:

$$Q_c = Q_{c,before} + 0,632 \cdot \Delta Q_c$$

From figure 6 one can read that this happens at about 4467 minutes of simulation time. One can also see that the response is delayed with just below 1 minute. This means that one has

$$\theta \approx 1min$$

and

$$\tau \approx 4467 - 4450 - \theta = 16min$$

For the holdup in V-100, which was assumed to be integrating ², the response to a step in the opening of VLV-100 is shown in figure 7.

For an integrating process, the steady-state gain is replaced with the slope divided by the step in input variable (recall from section 2.1.3 that $g(s) = k \frac{e^{\theta s}}{s}$ for an integrating process). From figure 7 one can read the slope that results from the step in the opening of VLV-100:

$$\frac{dm}{dt} = \frac{4,058kmol - 3,544kmol}{4253,6min - 4176,0min} = 6,624 \cdot 10^{-3} kmol/min$$

The slope must be scaled to get the value in % of the range:

$$\left(\frac{dm}{dt}\right)_{scaled} = \frac{6,624 \cdot 10^{-3}}{7.5} \cdot 100\% = 8,83 \cdot 10^{-2}\%/min$$

Finally, divide by the change in the input (Δz) to get k :

²For a level in a non-cyclic process this is always true, in a cyclic process it might not be

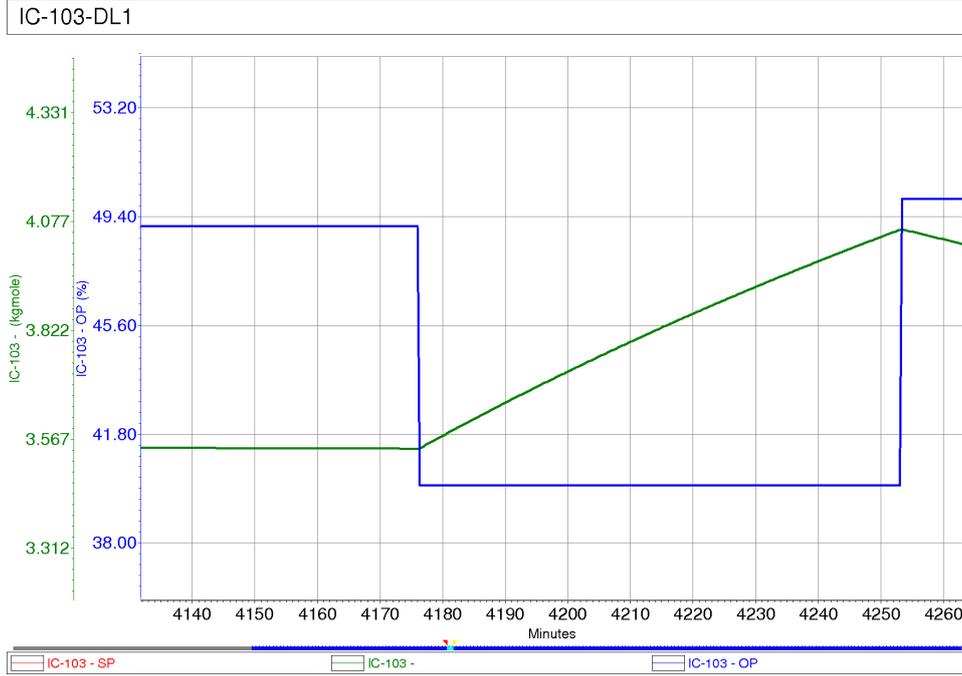


Figure 7: Response in controlled variable (V-100 holdup) to a step in manipulated variable (VLV-100 opening)

$$k = \frac{(dm/dt)_{scaled}}{\Delta z} = \frac{8,83 \cdot 10^{-2}\%}{9\%} = 9,81 \cdot 10^{-3}$$

The delay θ is read from the plot, and is $\approx 0,4min$.

The controller settings were found by using the SIMC rules as described in Skogestad's paper [4].

The transfer function parameters found by the step response testing are shown in table 7, the k values refer to the steady state gain from manipulated to controlled variable.

After tuning of the level and load controllers was done, the last manipulated variable (the % opening of VLV-103) was increased in 5 % steps from 50 to 100 % open to find the optimal valve opening, to be used as a nominal point for testing of the different control setups. The chosen nominal point was $z_{VLV-103} = 60\%$.

The three different choices of controlled variable for the last manipulated variable (VLV-103) required different tuning. For control of ΔT (case I) the step response from opening VLV-103 from 60 to 65 % was taken as basis for finding the transfer function parameters. The response is shown in figure 8.

The subcooling at the condenser outlet was also tracked during this simulation case, so the response to stepping in valve position was available

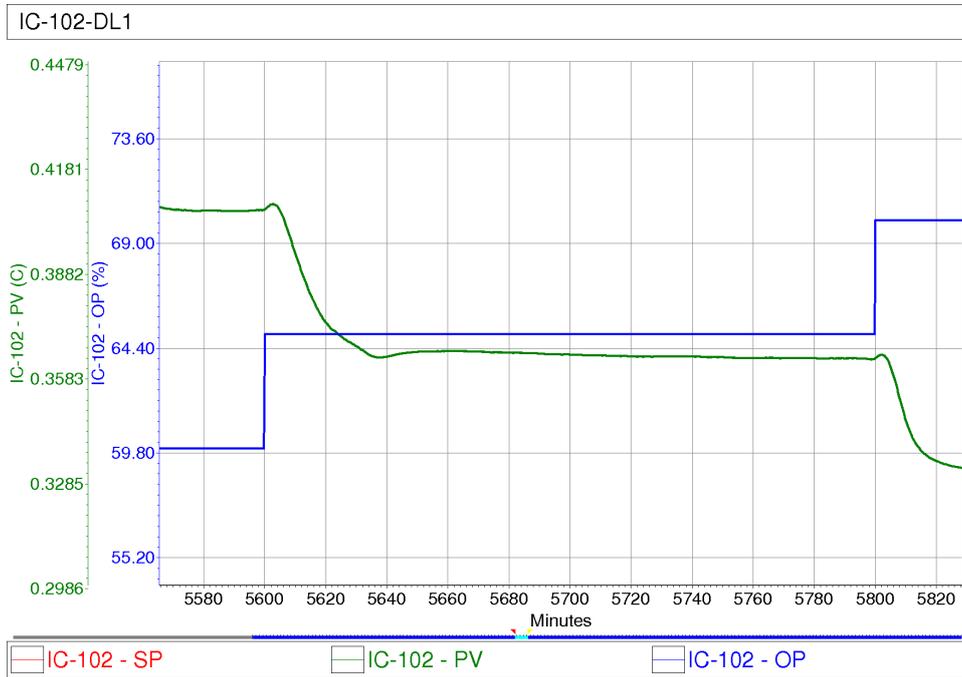


Figure 8: Response in ΔT to a step in opening of VLV-103 from 60 to 65 %

for the entire case. Figure 9 shows the response in ΔT_{sub} to the step in valve position from 60 to 65 % open.

The last variable that was tried as the third controlled variable was the pressure on the high-pressure side (P_h). Figure 10 shows the response in P_h to a step in valve position from 65 to 60 % open³.

Based on the responses shown in figures 8, 9 and 10, the transfer function parameters from opening of VLV-103 to the different variables to be controlled by this valve were calculated just like those for the Q_c and V-100 holdup controllers.

Table 7: Transfer function parameters

CV	Specified span	k	θ (min)	τ (min)
Q_c	$0-1.08 \cdot 10^4 \text{ kJ/h}$	1,61	1,0	16
Holdup	0–7,5 kmol	0,0098	0,4	–
ΔT	-1 – 4 °C	0,168	5	11
ΔT_{sub}	-1 – 19 °C	0,7	0.5	2,0
P_h	500 – 1500 kPa	0,36	0,5	1,8

According to the rules shown in table 1 and the transfer function param-

³The responses to steps 60-65 and 65-60 were slightly different - the latter would give the most conservative controller parameters and was therefore chosen.

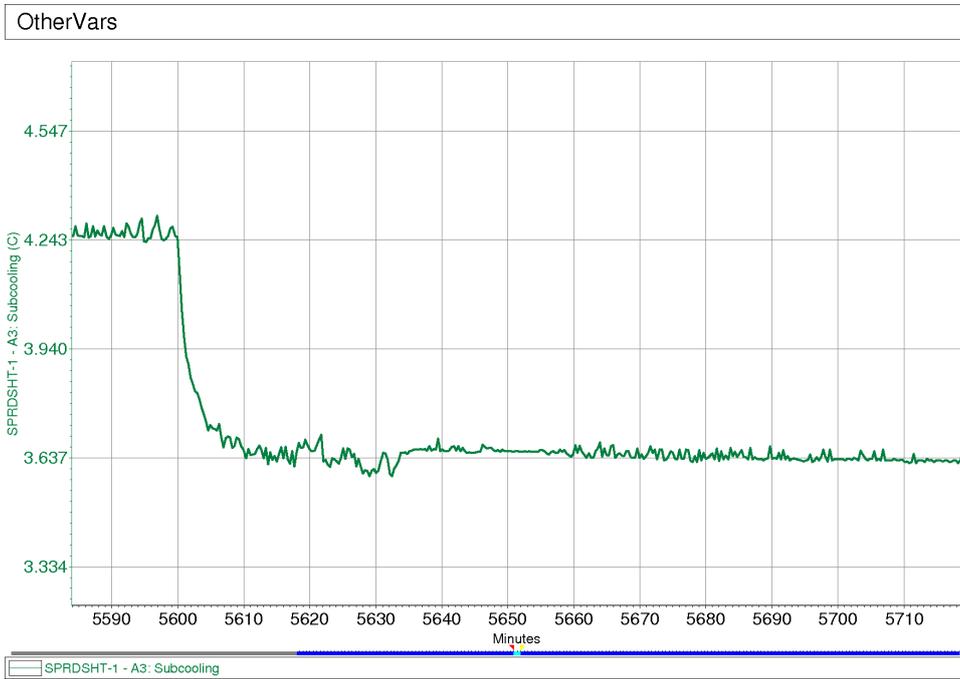


Figure 9: Response in subcooling to step in valve position from 60 to 65 % open

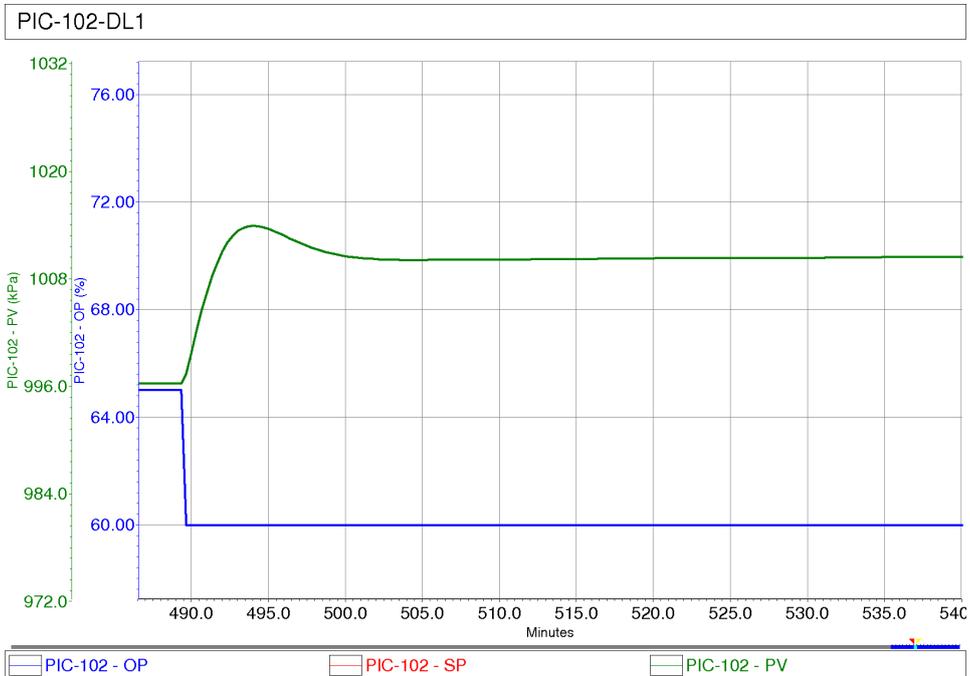


Figure 10: Response in P_h to step in valve position from 65 to 60 % open

eters shown in table 7, tuning parameters were decided for the controllers. The chosen parameters ⁴ are shown in table 8. The controller names refer to the HYSYS flowsheet as shown in figure 4. After the controller settings were determined, the control setup was tested by simulating different disturbance scenarios, described in the next section (3.7).

Table 8: PID controller settings from SIMC tuning rules

Controller	K_c	τ_I
IC-102 (ΔT)	4,37	11,0
IC-102 (ΔT_{sub})	1,90	2,00
IC-102 (P_h)	3,33	1,80
IC-103	127.4	–
IC-105	4,97	8,00

⁴For the load and level controllers, τ_c was set equal to θ , for the ΔT controller it was set to 2θ .

3.7 Testing of the control setup

3.7.1 Disturbances tested on the model

For each case, the following disturbances were introduced:

- A slow, linear increase in T_h from 20°C to approximately $22,5^\circ\text{C}$
- A step in T_h back to 20°C
- Changes in the set point for Q_c (set point for IC-105), from nominal value of $5,4 \cdot 10^4$ to $7,0 \cdot 10^4 \text{kJ/h}$ in two steps and then down to $5,4 \cdot 10^4$ in two steps
- A step in T_c from -10°C to -12°C , followed by a step back to -10°C
- New steps in the set point for Q_c , this time down to $4,8 \cdot 10^4$ and back to $5,4 \cdot 10^4$
- Steps in the set point for the last controlled variable

Between each disturbance, the process was given time to stabilize.

3.7.2 Case I, control of ΔT

Before the first disturbance was introduced, the integration was allowed to run until 43 minutes to stabilize completely.

For the time period where T_h was increased linearly, the controller responses are shown in figures 11, 12 and 13. The increase was started at 43 minutes and ended at 193 minutes. Figure 14 shows how T_h was varied. One can particularly notice how small the input usage is for the level controller, especially compared to the ΔT controller which responds quite hard when the disturbance occurs.

At 193 minutes, T_h was stepped back down to the nominal value. This is a large step compared to the nominal value of the condenser ΔT_{min} . The response to this step for the ΔT controller is shown in figure 15. This disturbance is the one with the largest response from IC-102, but the disturbance is also large compared to both the specified range of the controlled variable and to its absolute value.

Next, the set point for the cooling load (from here abbreviated $Q_{c,s}$) was stepped up to $6 \cdot 10^4 \text{kJ/h}$ (after 348 minutes), ramped up to $7 \cdot 10^4 \text{kJ/h}$ (between 423 and 428 minutes), ramped down to $6,2 \cdot 10^4 \text{kJ/h}$ (between 485 and 489 minutes) and returned to the nominal value at 570 minutes. Figure 16 shows how the Q_c controller tracked these set point changes. The response from the ΔT controller (IC-102) to these changes in $Q_{c,s}$ is shown in figure 17. One should notice that with $Q_{c,s} = 7 \cdot 10^4 \text{kJ/h}$ the ΔT controller reached saturation before the controlled variable had completely returned

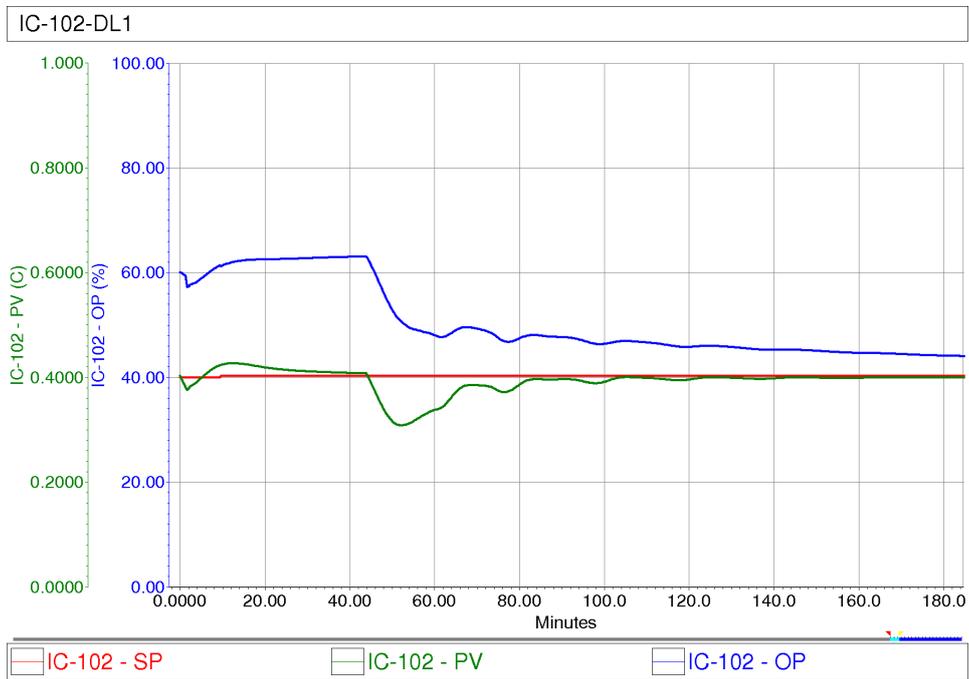


Figure 11: Response to a linear increase in T_h for ΔT controller IC-102

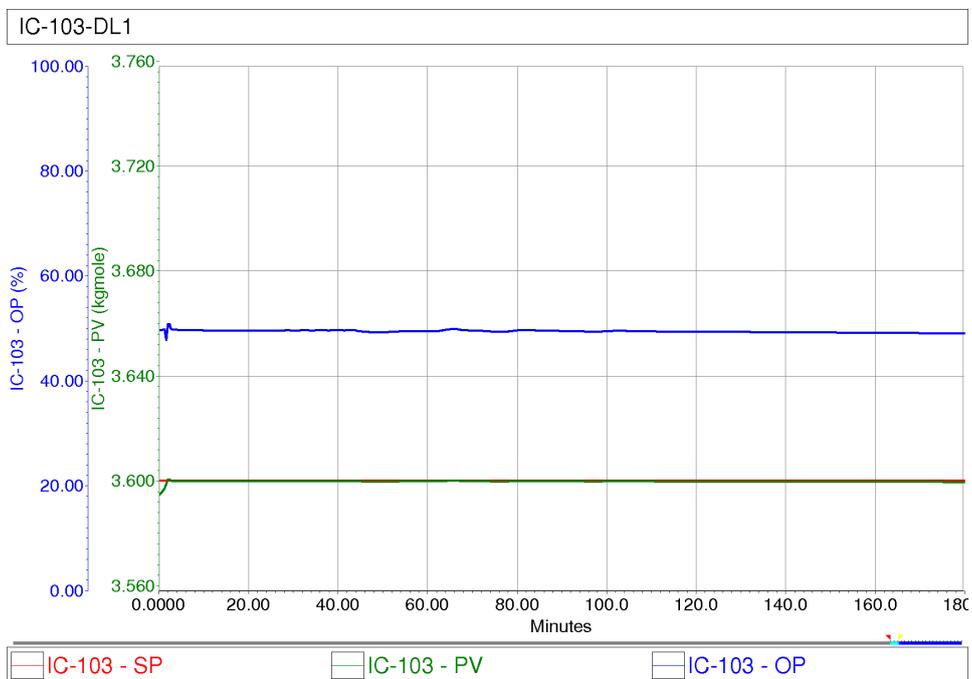


Figure 12: Response to a linear increase in T_h for level controller IC-103

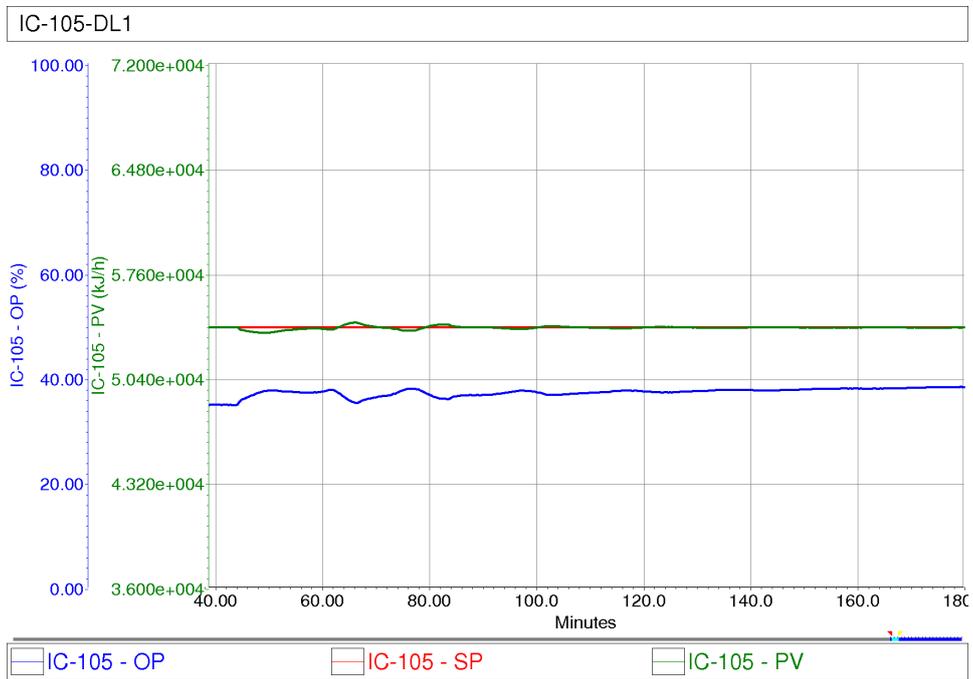


Figure 13: Response to a linear increase in T_h for load controller IC-105

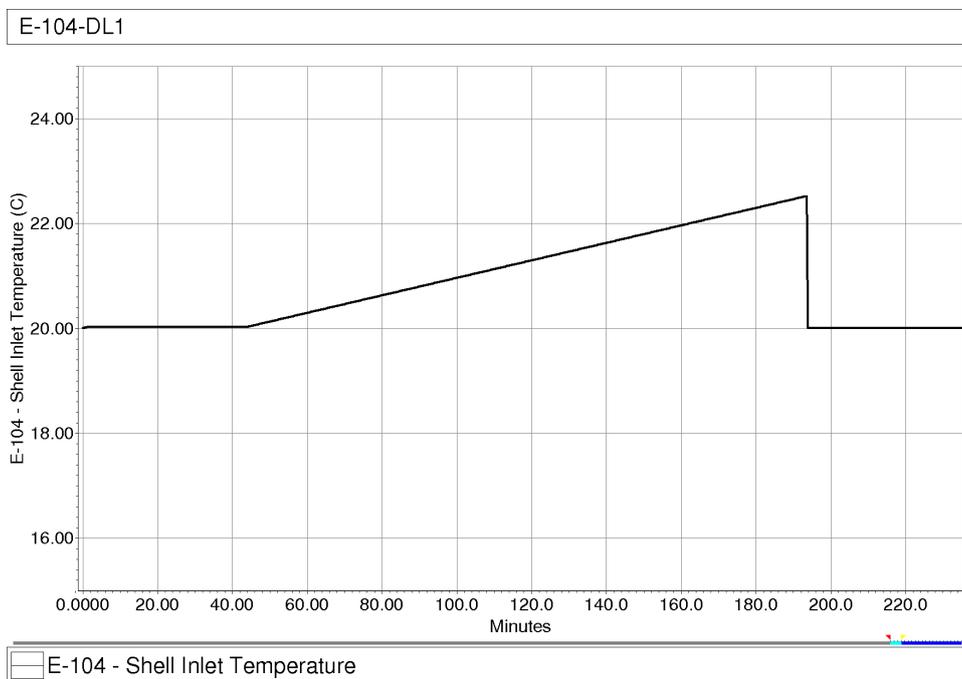


Figure 14: Disturbance in T_h , condenser shell inlet temperature

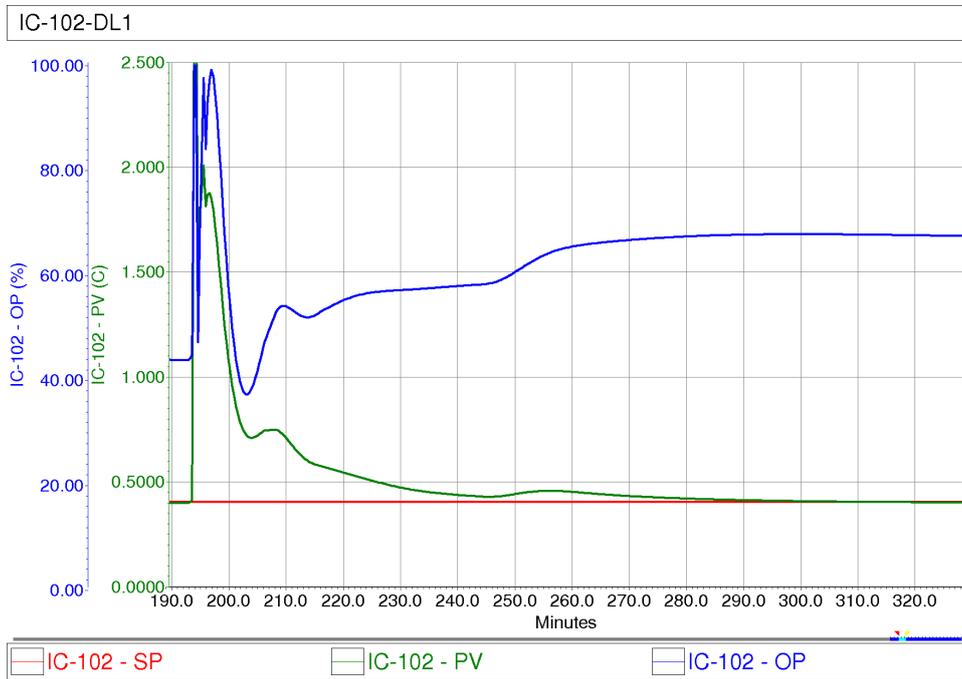


Figure 15: Response to a step in T_h for ΔT controller IC-102

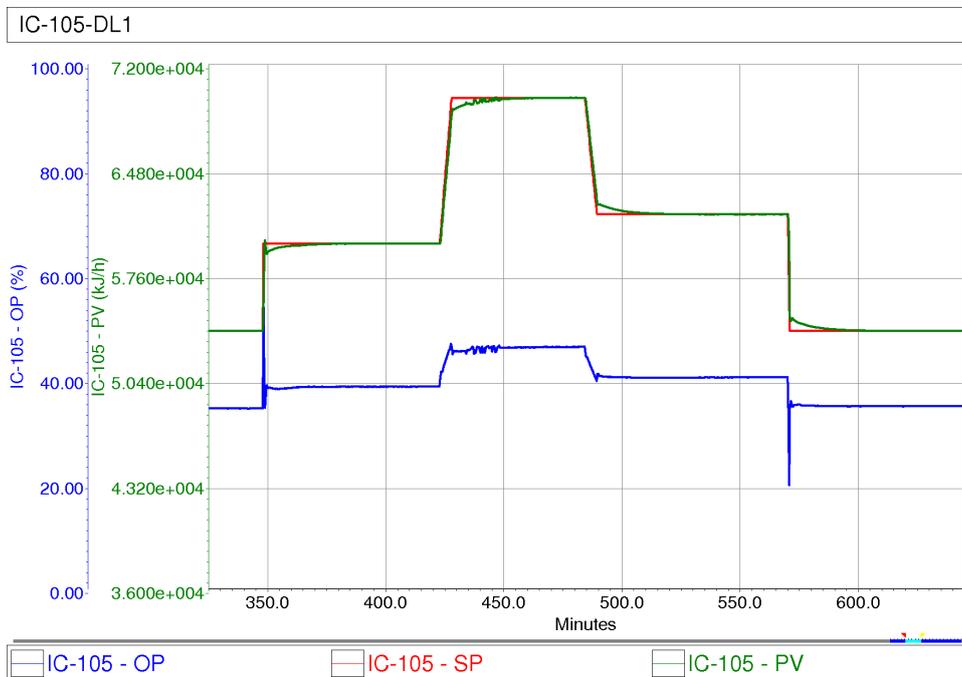


Figure 16: Response to steps in $Q_{c,s}$ for Q_c controller IC-105

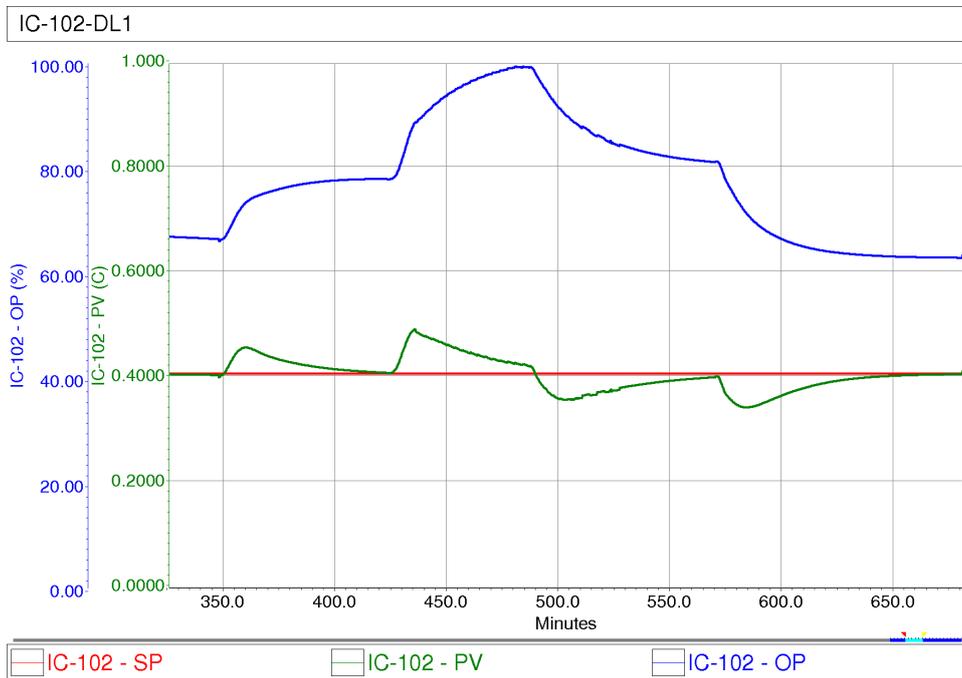


Figure 17: Response to steps in $Q_{c,s}$ for ΔT controller IC-102

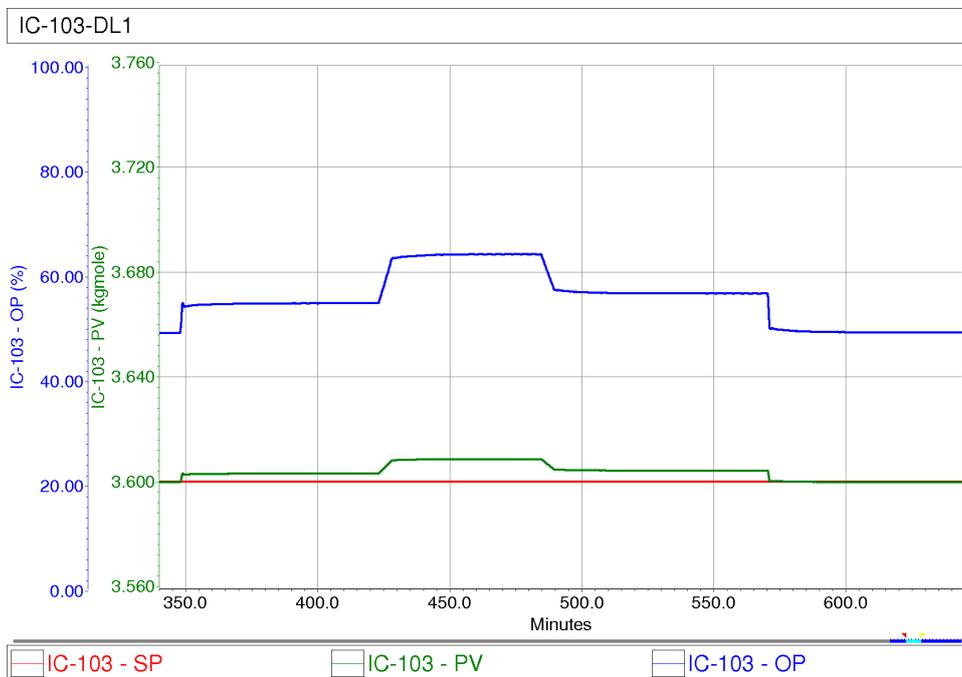


Figure 18: Response to steps in $Q_{c,s}$ for level controller IC-103

to its set point. For the changes in $Q_{c,s}$ the level controller also had to take some action, this is shown in figure 18

The next disturbance the control setup was tested for, was a decrease in T_c to -12°C after 680 minutes followed by an increase back to the nominal value at 756 minutes. The disturbance is shown in figure 19. The responses to this from the ΔT controller is shown in figure 20.

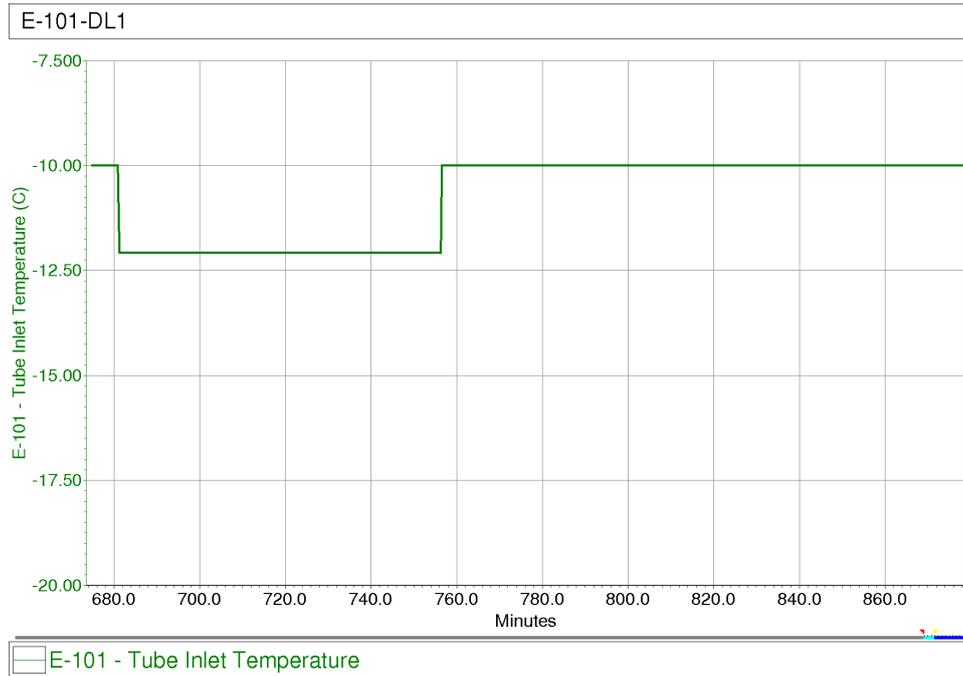


Figure 19: Steps in T_c

Then the set point for Q_c was reduced to $4,8 \cdot 10^4 \text{kJ/h}$ at 1200 minutes and returned to $5,4 \cdot 10^4 \text{kJ/h}$ at 1268 minutes. Figure 21 shows how the set point change was tracked by the Q_c controller and 22 shows how the ΔT controller responded.

At 1357 minutes the set point for ΔT was increased to $0,4533^\circ\text{C}$, and returned to $0,4033^\circ\text{C}$ after 1410 minutes. Figure 23 shows how the set point changes were tracked by the ΔT controller. The control seems to be quick and smooth.

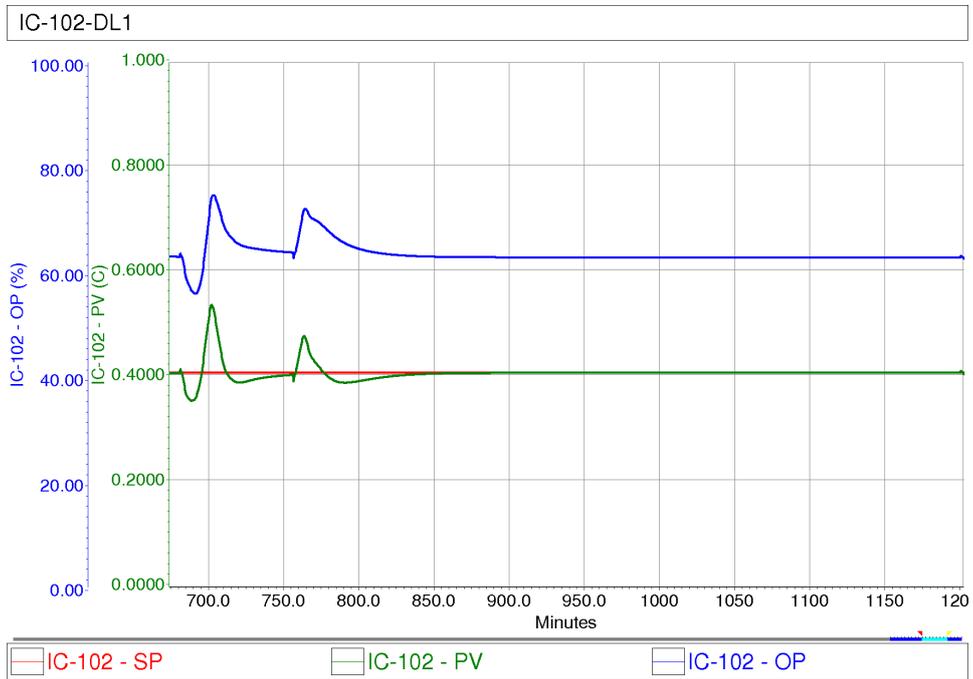


Figure 20: Response to steps in T_c for ΔT controller IC-102

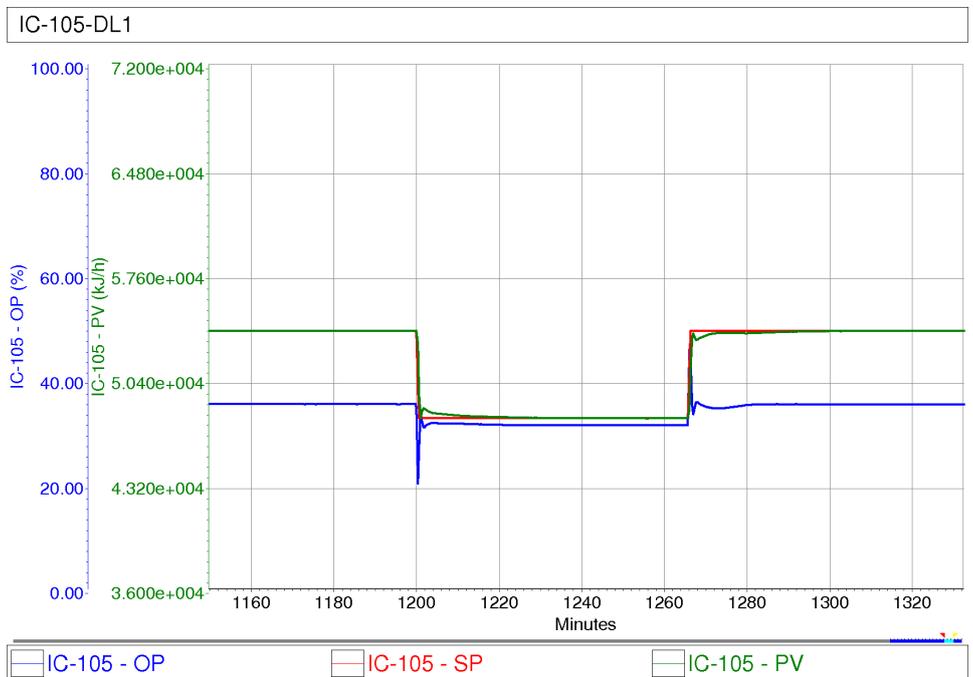


Figure 21: Response to steps in $Q_{c,s}$ for Q_c controller IC-105

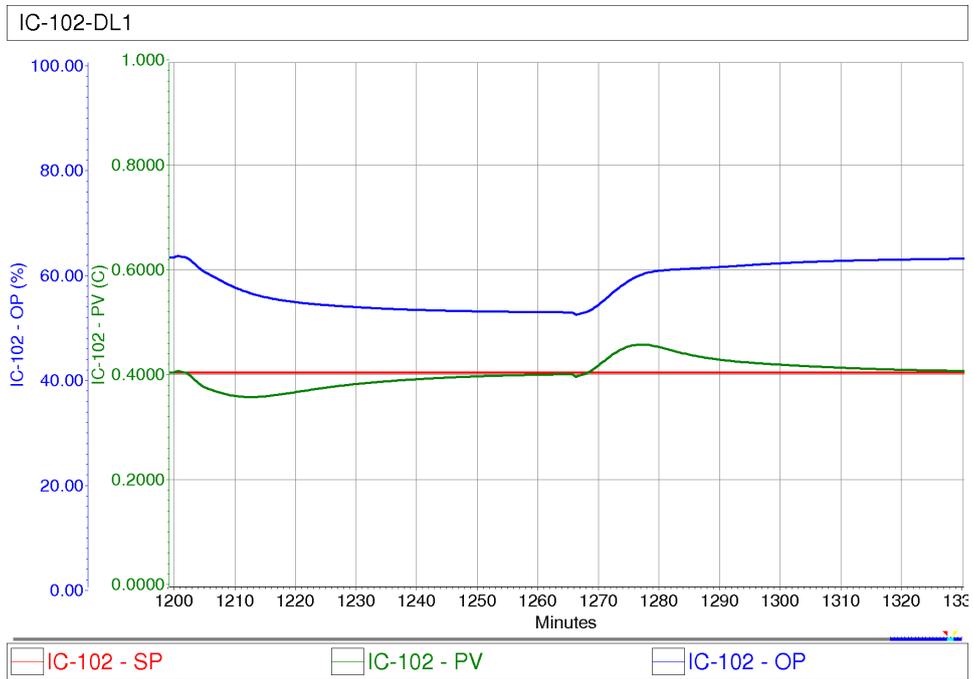


Figure 22: Response to steps in $Q_{c,s}$ for ΔT controller IC-102

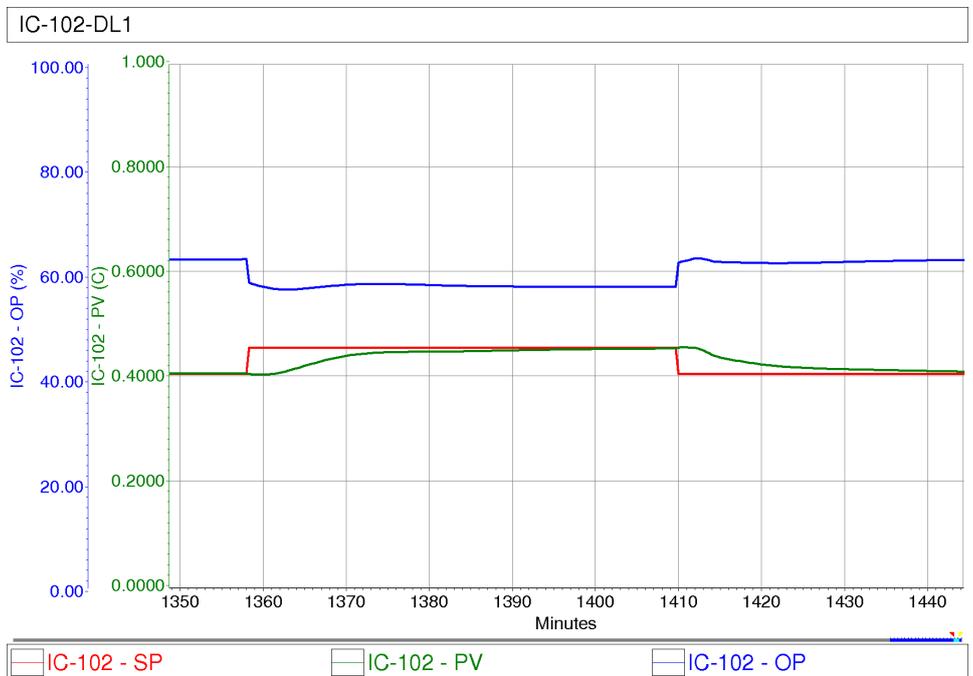


Figure 23: Response to steps in ΔT_s for ΔT controller IC-102

3.7.3 Case II, control of ΔT_{sub}

The period of linear increase in T_h lasted from 85 to 253 minutes. The disturbance is illustrated in figure 24, the response from the ΔT_{sub} controller, IC-102, is shown in figure 25. It seems as the control action is much smoother than for control of ΔT (compare with figure 11).

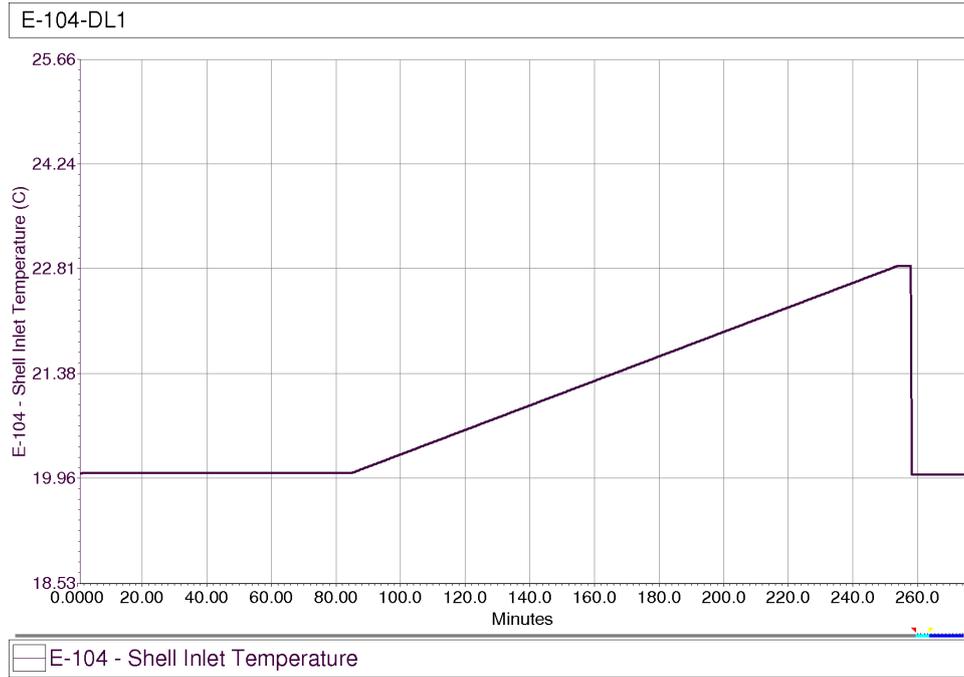


Figure 24: Shows the linear increase in T_h and the step back to nominal value

Figures 26 and 27 show the responses from the two other controllers (IC-103 and IC-105) to the same disturbance. One can particularly notice that the level controller hardly needs to take any action at all.

The step in T_h back to 20°C was done at 253 minutes, and figure 28 shows how the ΔT_{sub} controller responded to this step. The controller response seems smooth, but the time required for the manipulated variable (z for valve VLV-103) to stabilize is rather long.

Figure 29 illustrates how the ΔT_{sub} controller responded to the stepwise changes in the set point for the Q_c controller, beginning at 485 minutes. It is worth noticing that the responses to the first and last steps seem less smooth than for the other two step. This may be because the first change in $Q_{c,s}$ is a step while the other changes are 'ramps', i. e. the set point is changed over a short period of time instead of instantaneously. The last ramping is done faster than the two before it, and is closer to an instantaneous step. Figure 30 shows the set point changes and how the Q_c controller handled

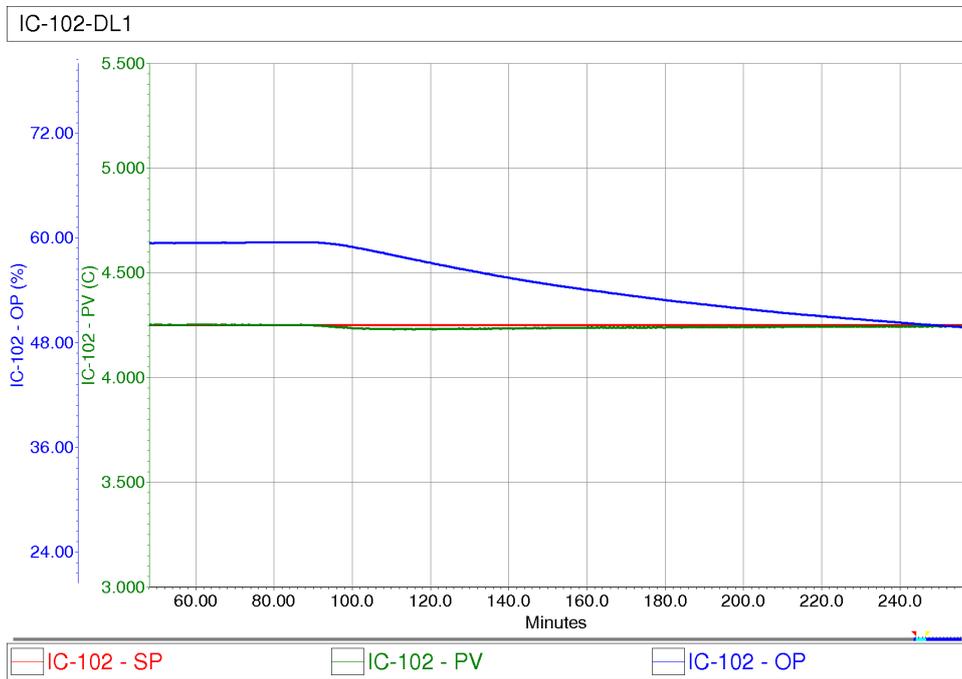


Figure 25: Response to a linear increase in T_h for ΔT_{sub} controller IC-102

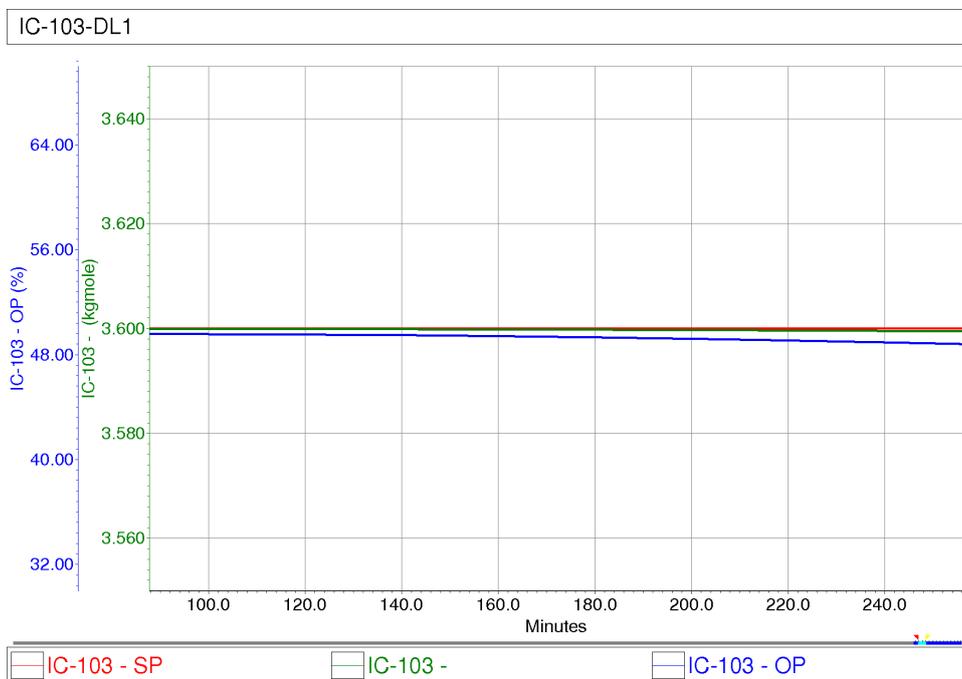


Figure 26: Response to a linear increase in T_h for level controller IC-103

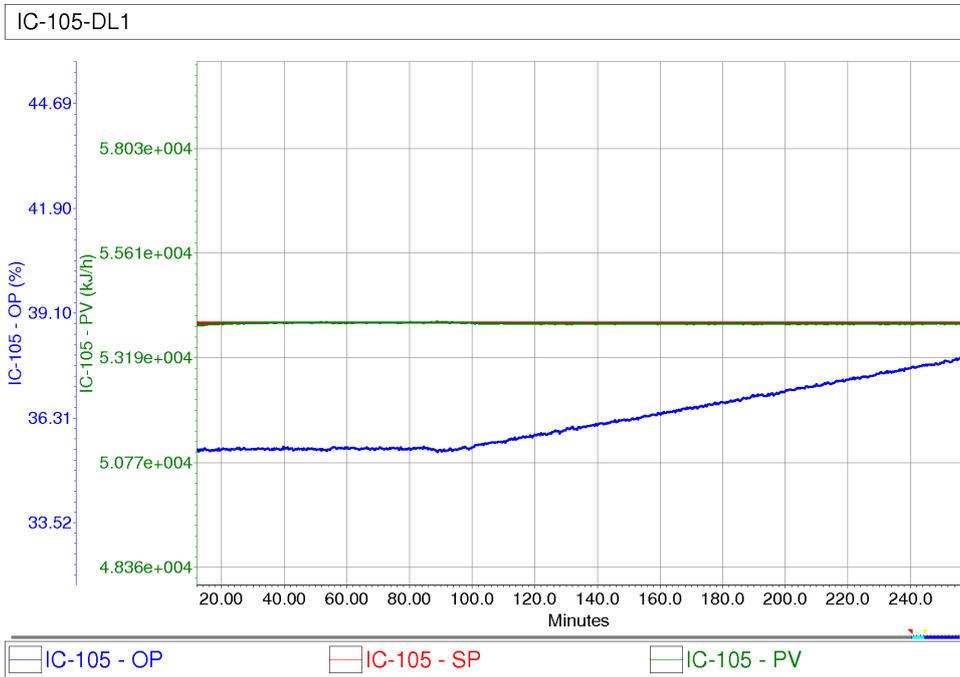


Figure 27: Response to a linear increase in T_h for Q_c controller, IC105

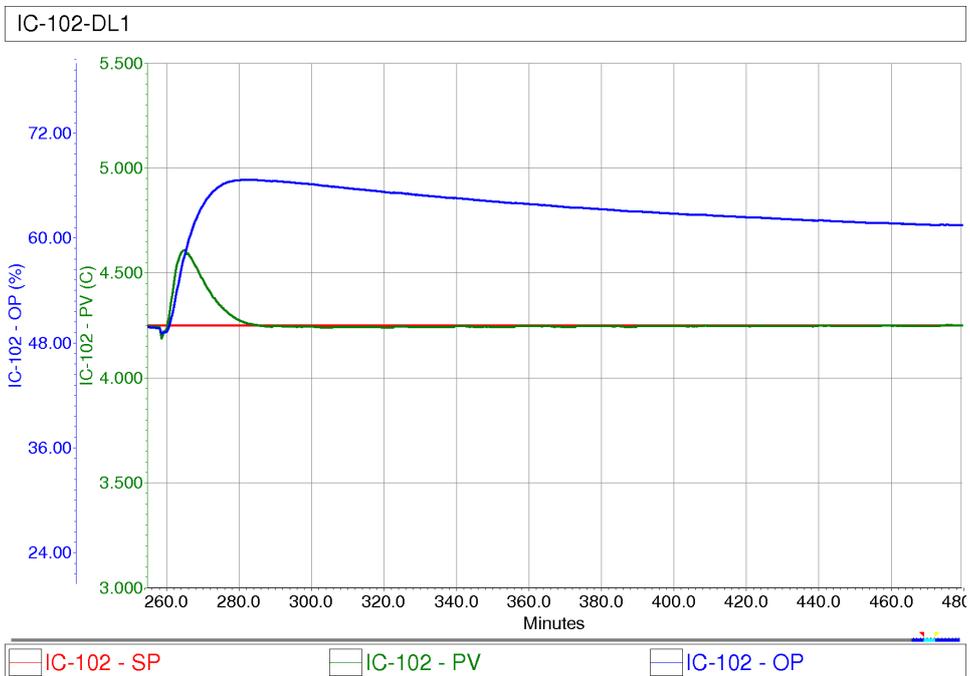


Figure 28: Response to a step in T_h for ΔT_{sub} controller IC-102

these changes. One can notice the rough behaviour from the Q_c controller to the change in set point from $6 \cdot 10^4$ to $6 \cdot 10^4$ kJ/h. A possible explanation is given in section 3.8.3.

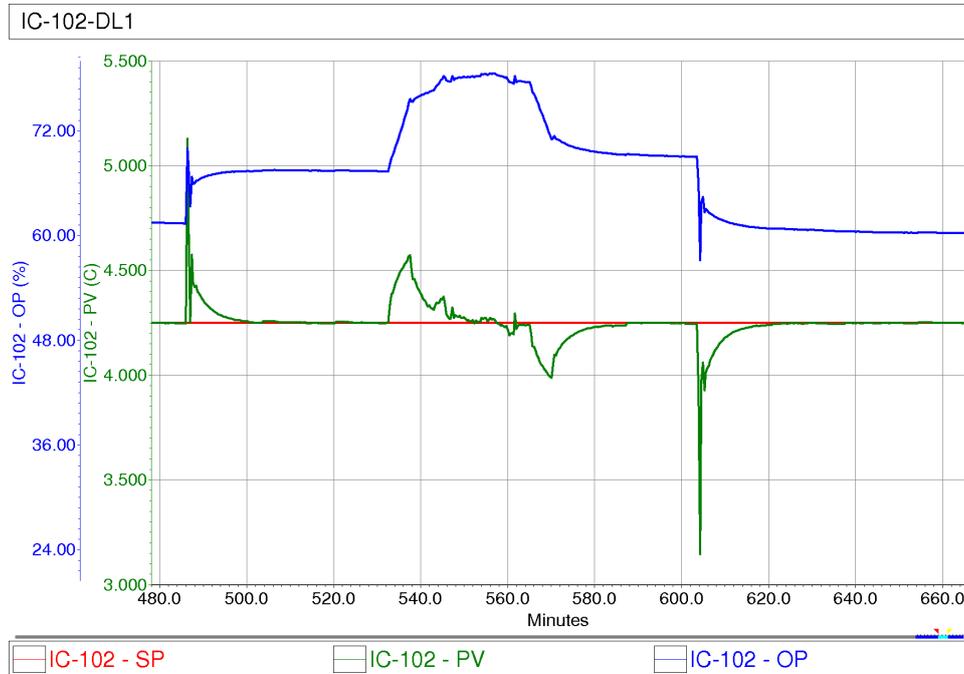


Figure 29: Response to changes in $Q_{c,s}$ for ΔT_{sub} controller IC-102

Figure 31 shows how the ΔT_{sub} controller responded to the stepwise changes in T_c after 667 and 735 minutes. The disturbance itself is illustrated in figure 33. This is actually the disturbance that causes the largest action from the ΔT_{sub} controller. This is best understood as a result of the Q_c controller also having to respond forcefully - after all, the driving force in the vaporizer is reduced by 40 % by this step and the compressor power must increase significantly to handle this (illustrated by figure 32 which shows the response from the Q_c controller).

At 809 minutes the set point for Q_c was ramped down to $4,8 \cdot 10^4$ kJ/h, before it was returned to $5,4 \cdot 10^4$ kJ/h at 834 minutes. The responses from the ΔT_{sub} and Q_c controllers are shown in figures 34 and 35. Both controllers handle this disturbance easily.

The final disturbance done to the process was to change the set point for ΔT_{sub} from $4,25^\circ\text{C}$ to $4,75^\circ\text{C}$ at 865 minutes before returning it to $4,25^\circ\text{C}$ at 885 minutes. Figure 36 shows the set point changes and how the ΔT_{sub} controller responded. The figure shows that the input usage was smaller here than for any of the other disturbances even though $\Delta T_{sub,s}$ is further from the nominal value than ΔT_{sub} actually was for several other disturbances.

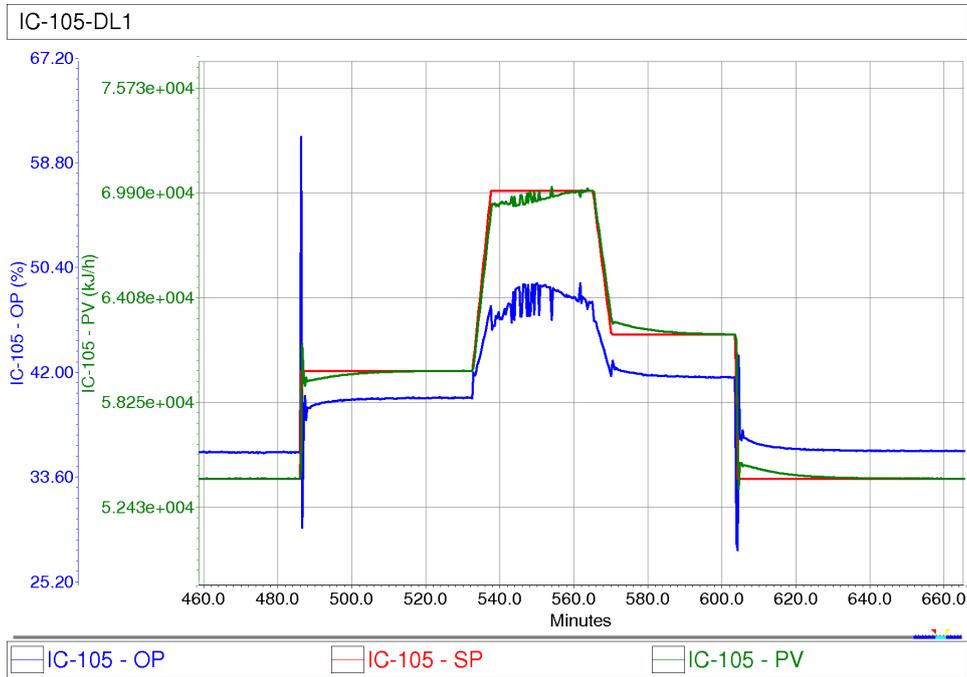


Figure 30: Set point changes for Q_c controller IC-105

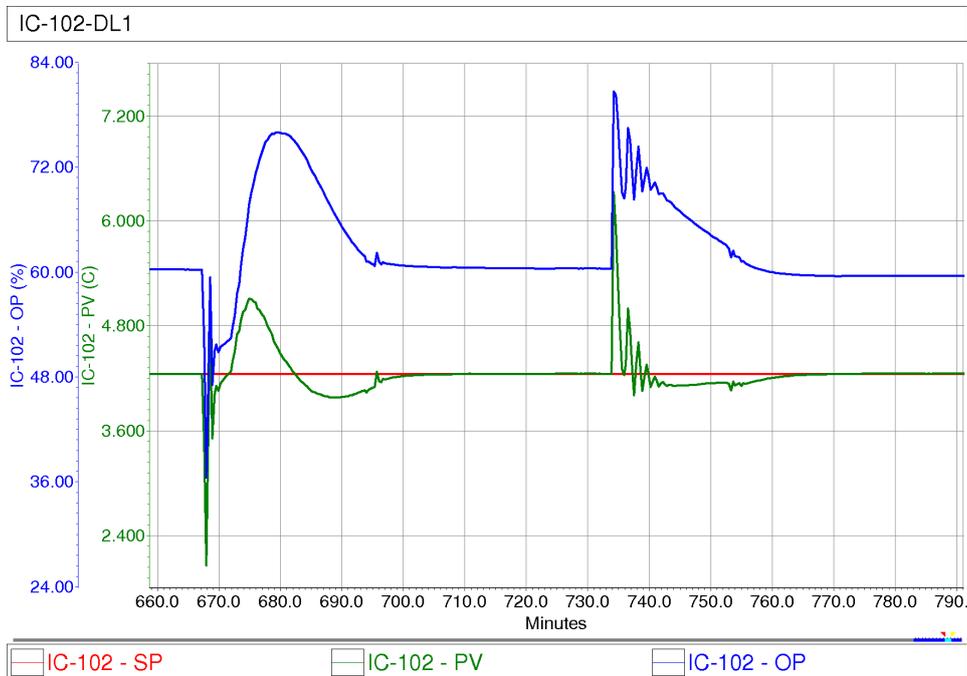


Figure 31: Response to changes in T_c for ΔT_{sub} controller IC-102

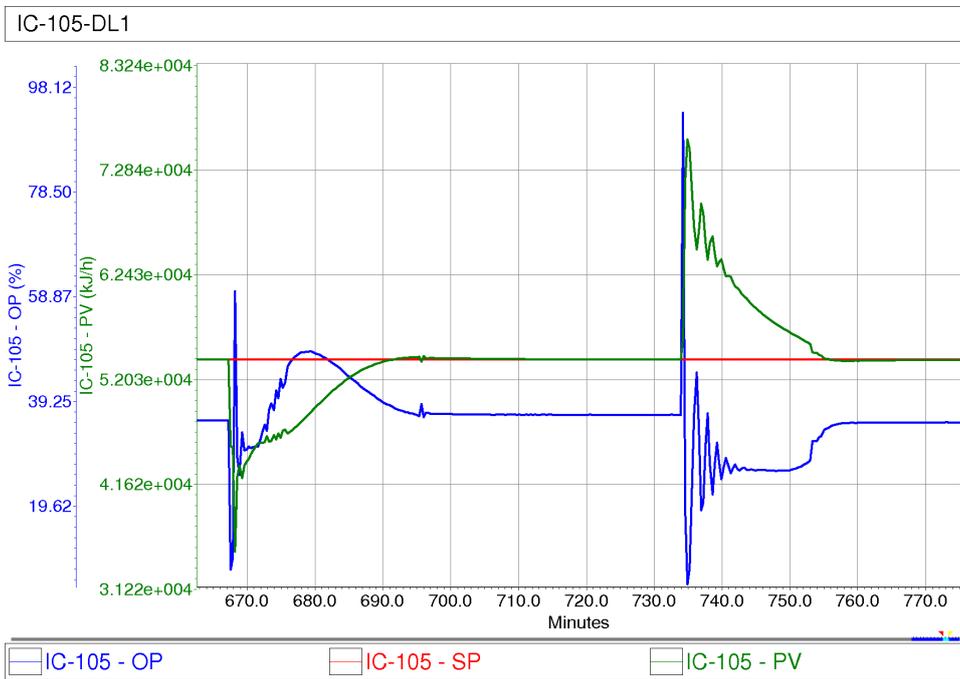


Figure 32: Response to changes in T_c for Q_c controller IC-105

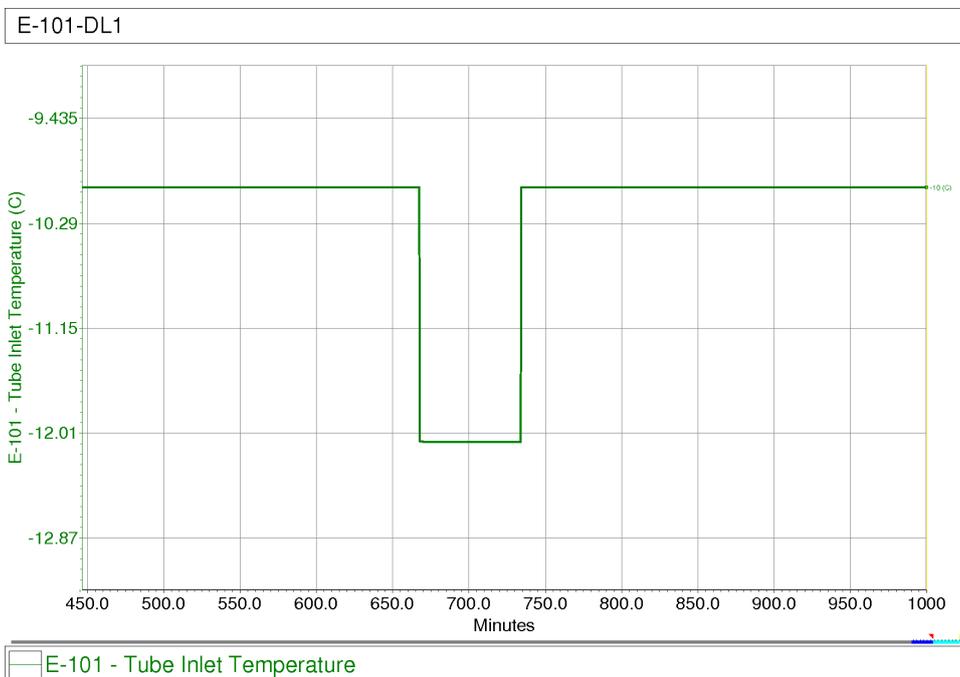


Figure 33: Stepwise changes in T_c (tube inlet temperature in vaporizer)

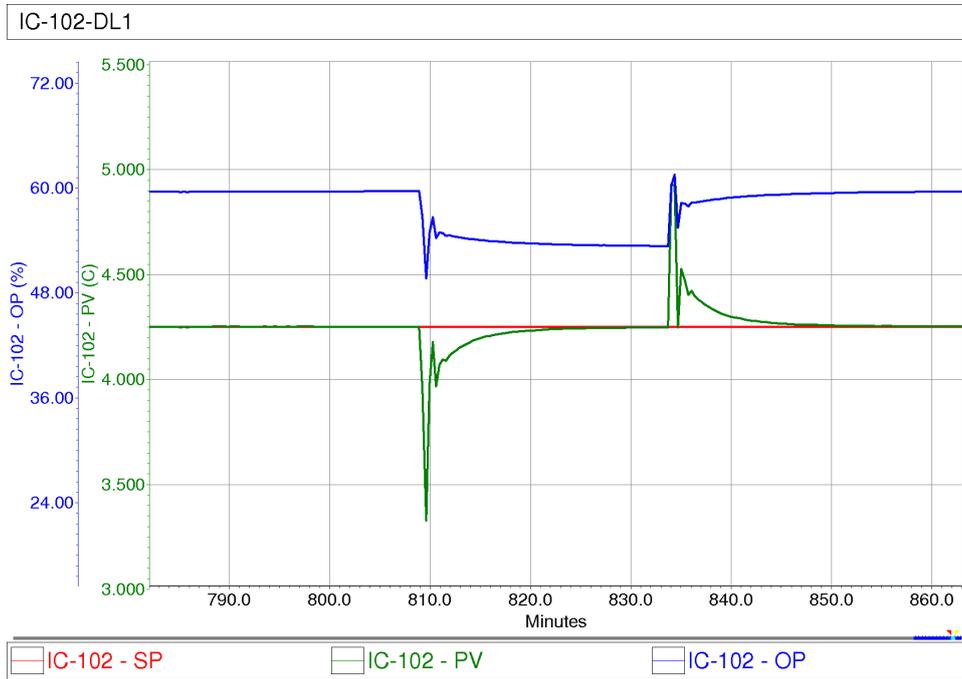


Figure 34: Response to changes in $Q_{c,s}$ for ΔT_{sub} controller IC-102

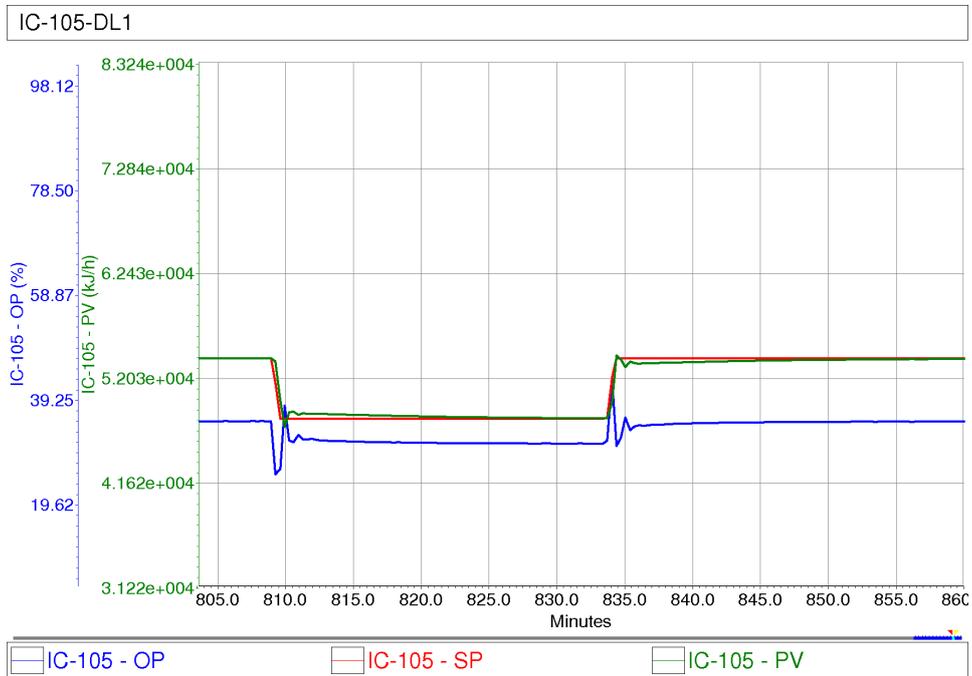


Figure 35: Response to changes in $Q_{c,s}$ for Q_c controller IC-105

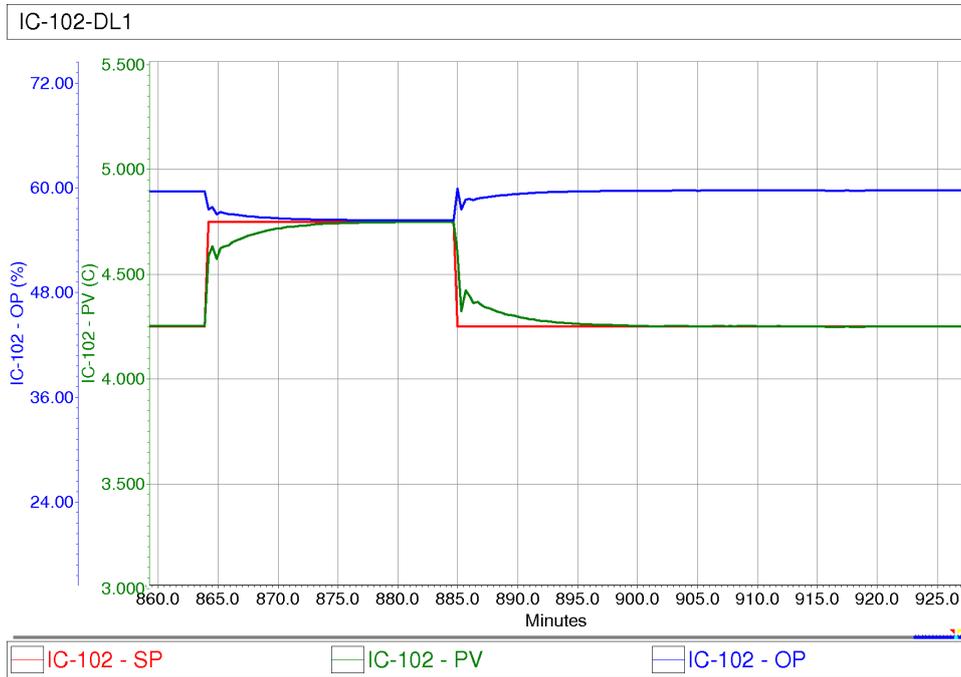


Figure 36: Response to changes in $\Delta T_{sub,s}$ for ΔT_{sub} controller IC-102

3.7.4 Case III, control of P_h

The first disturbance introduced was again the linear increase in T_h (see figure 37), starting at 135 minutes and stopping at 280 minutes. The response from the pressure controller is shown in figure 38. The increase in temperature was stopped after 190 minutes.

Figure 39 shows the response from the pressure controller to the step in T_h back to 20°C after 288 minutes, and figure 40 shows the response from the Q_c controller.

The same changes were made to $Q_{c,s}$ as in the two previous cases. The changes were done at 350, 406, 444 and 516 minutes; figure 41 shows the set point changes and the response from the Q_c controller, figure 42 shows how the pressure controller responded. Notice that the same small ‘spikes’ are observed here as for the disturbance in T_c in the case with ΔT_{sub} control. Again, see section 3.8.3 for a possible explanation. It should also be noticed that the pressure P_h did not get back to the set point until the set point for Q_c had been reduced to $6,2 \cdot 10^4$ kJ/h.

The next disturbance was a change in T_c down to -12°C after 570 minutes and back to -10°C after 615 minutes. Figure 43 shows the disturbance and figure 44 shows how the pressure controller responded to these disturbances. The valve went to fully open also for this disturbance (but for a shorter time than for the step in T_h)

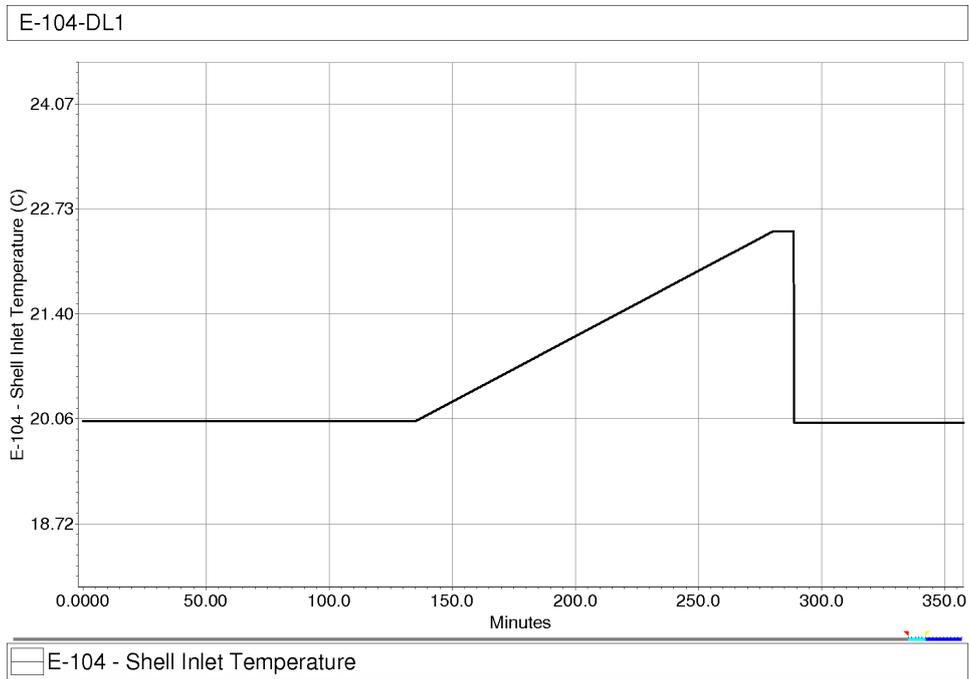


Figure 37: Shows the linear increase in T_h and the step back to nominal value for Case III

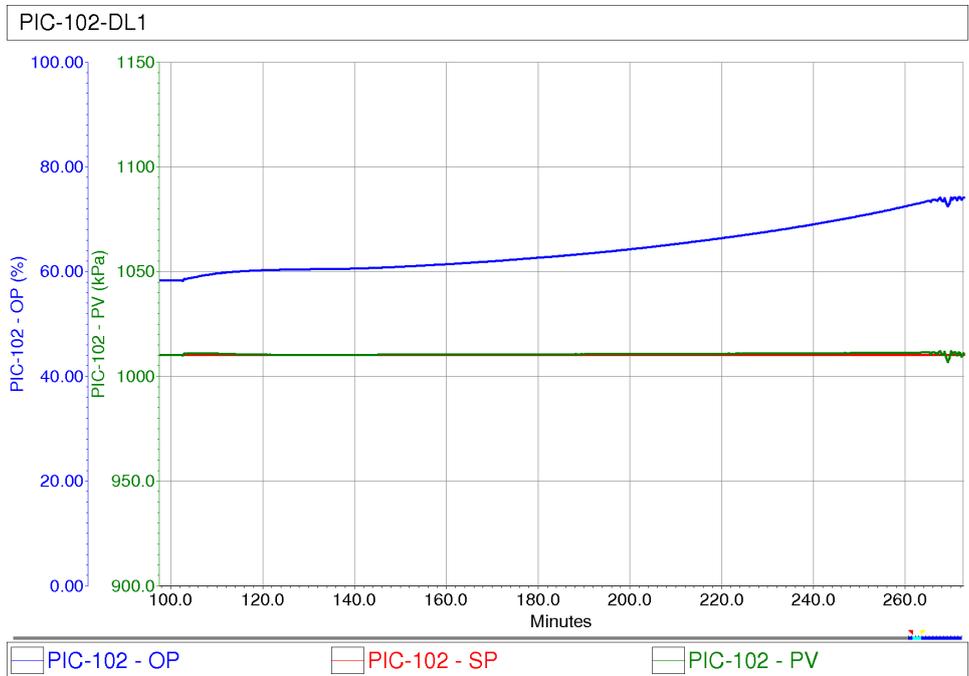


Figure 38: Response to a linear increase in T_h for P_h controller, PIC-102

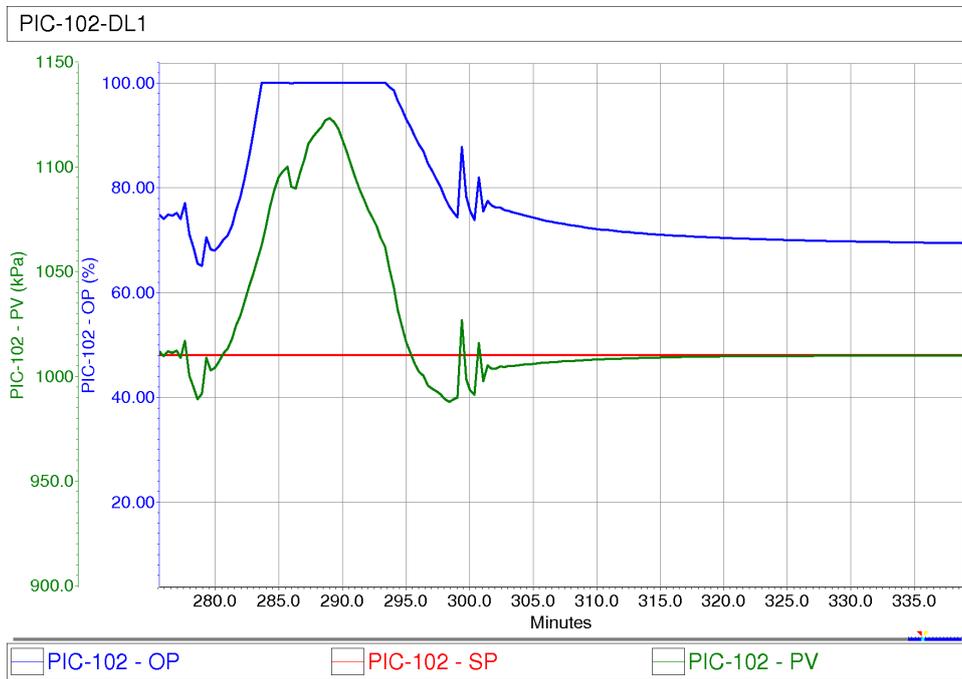


Figure 39: Response to a step in T_h for P_h controller, IC-102

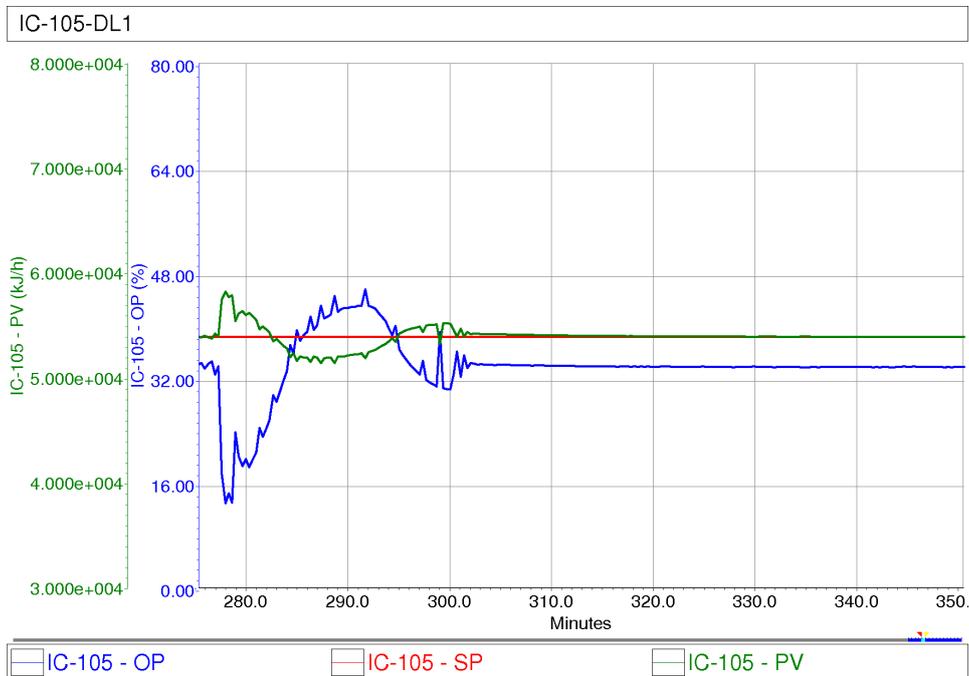


Figure 40: Response to a step in T_h for Q_c controller, IC-105

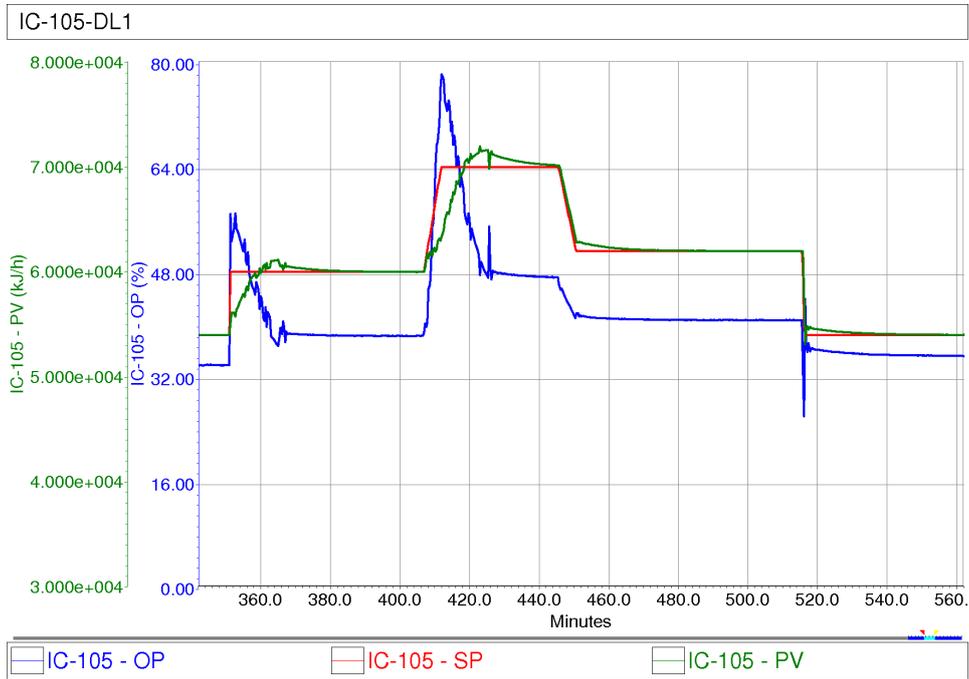


Figure 41: Response of Q_c controller, IC-105, to stepwise changes in $Q_{c,s}$

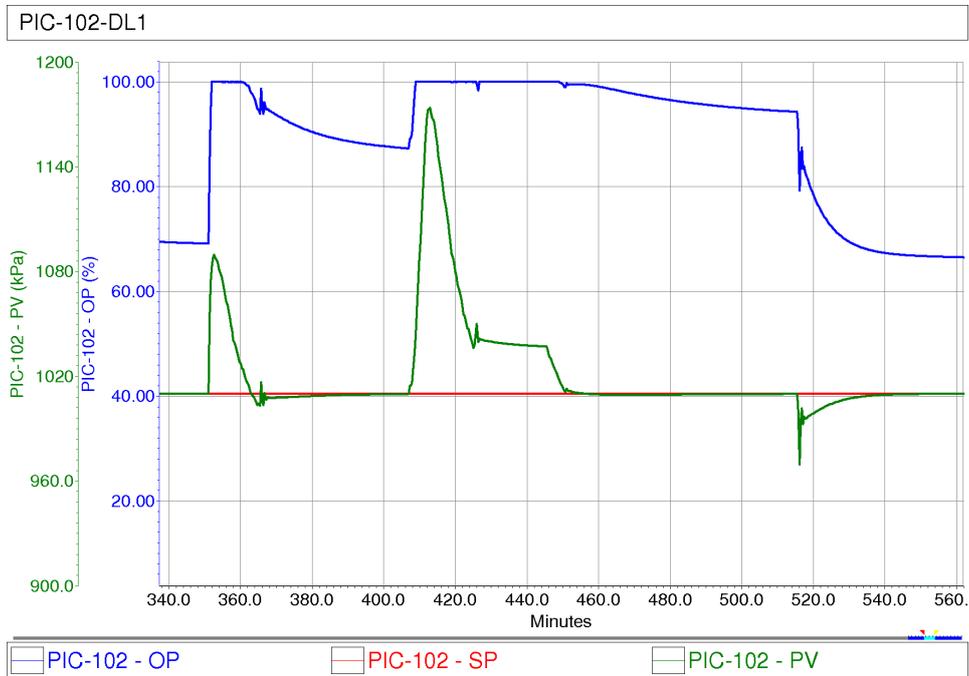


Figure 42: Response of P_h controller, IC-102, to stepwise changes in $Q_{c,s}$



Figure 43: Stepwise changes in T_c (tube inlet temperature in vaporizer)

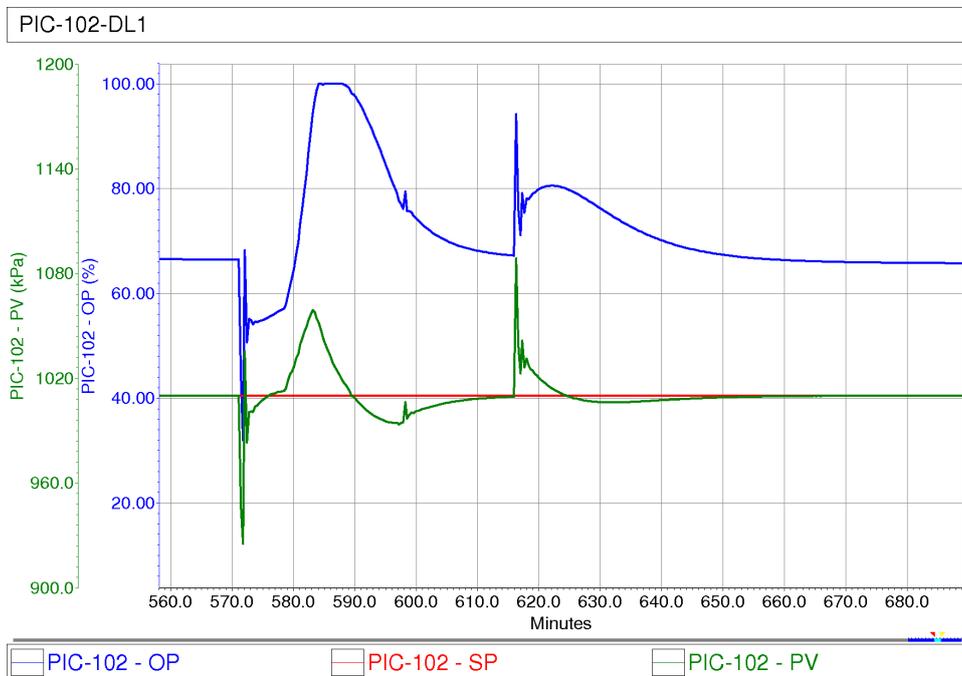


Figure 44: Response of P_h controller, IC-102, to stepwise changes in T_c

The set point for Q_c was again ramped down to $4,8 \cdot 10^4 kJ/h$ (at 689 minutes) before returning it to $5,4 \cdot 10^4 kJ/h$ at 730 minutes. Figures 45 and 46 show the responses from the P_h and Q_c controllers, respectively. This change was handled smoothly by the controllers.

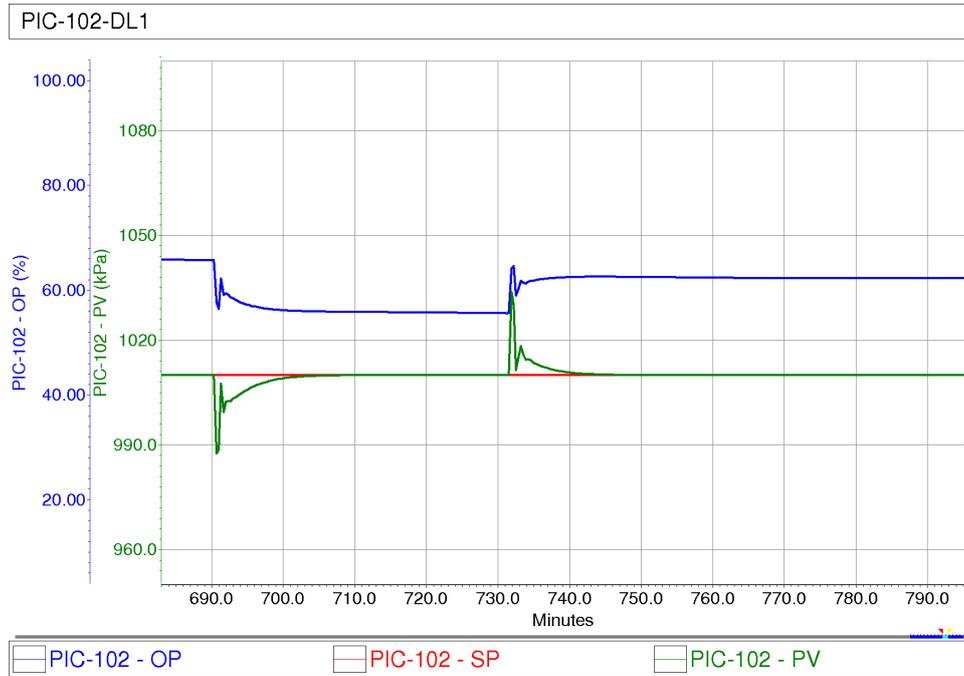


Figure 45: Response to changes in $Q_{c,s}$ for P_h controller PIC-102

The last disturbance was a set point change for the P_h controller, from 1010 kPa to 1060 kPa at 800 minutes and back to 1010 kPa at 852 minutes. Figure 47 shows how the controller responded to these set point changes. The set point tracking was rather fast and smooth, which indicates that the controller was properly tuned.

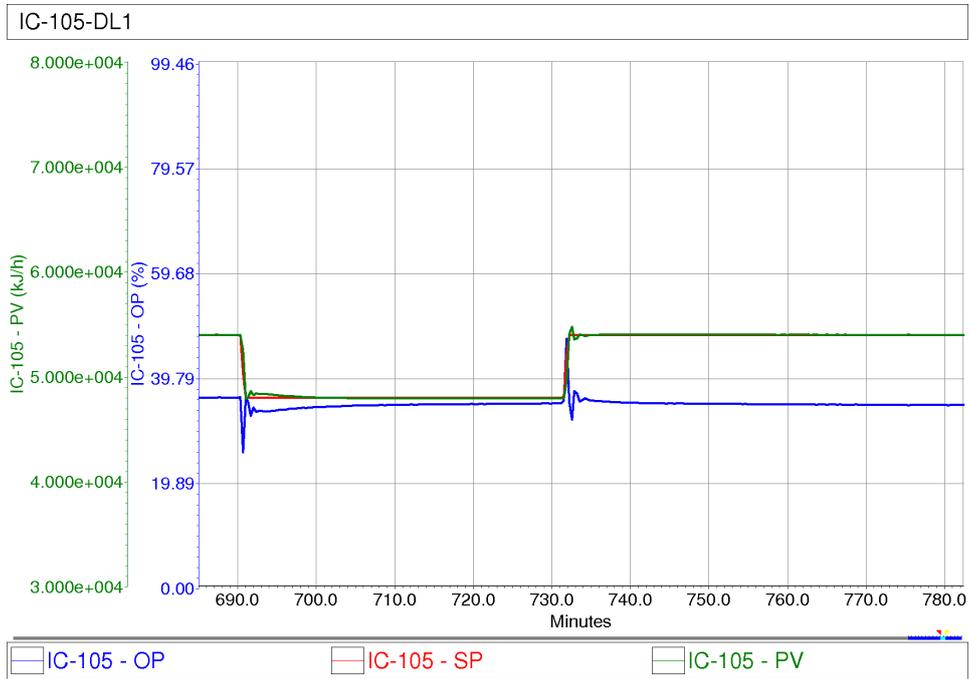


Figure 46: Response to changes in $Q_{c,s}$ for Q_c controller IC-105

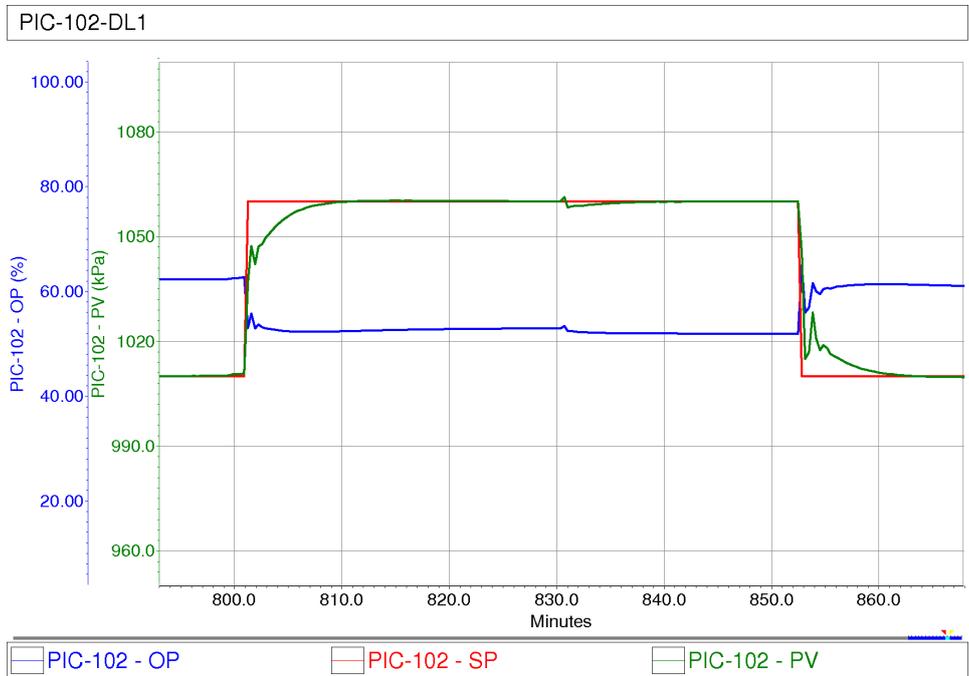


Figure 47: Response to changes in $P_{h,s}$ for P_h controller PIC-102

3.8 Discussion of results

3.8.1 Modelling

One drawback with the HYSYS software is how holdups in heat exchangers are initialized. In a real process, there will typically be both liquid and vapour present in vaporizers and condensers. In dynamic HYSYS simulations, the initial holdup will have the same properties (temperature, pressure, composition, vapour fraction) as the product leaving the exchanger, or a stream chosen by the user. It is not possible to specify an initial liquid level or a number of moles. When the process stabilizes after startup, there will usually be both liquid and vapour present. This means that the holdup(s) initially specified for the liquid tank(s) in the process will not be equal to the ones at which the process will stabilize. In this case, the low-pressure tank V-101 stabilized at approximately 47 % full with liquid - the remaining liquid having accumulated in the condenser. If one of the holdup levels is controlled and the other is not, the uncontrolled holdup should contain enough fluid to fill the heat exchangers without the tank itself running empty.

3.8.2 Optimization

The simulations carried out show that subcooling at the condenser outlet would be optimal, see table 6. The numerical value is different from the study by Jensen and Skogestad [1], but this is not important - the optimal value that is found using a simulation program will depend on the model equations and parameters used for the different unit operations. Especially how the heat exchangers are modelled, will strongly affect the exact values found.

It should be noticed that the optimum found was very flat - figure 5 shows a minimum at approximately 80 % open valve, but the minimum value is not much smaller than the value for a 100 % open valve.

Initially a simulation was carried out where the basic rating model (UA specified and end-point calculation) was used for the condenser. This simulation did actually not show any optimum - as shown by table 9 the compressor power was smallest for the largest valve opening (Z) for VLV-103.

The simulations carried out clearly illustrate the significance of the kind of model used for heat exchangers. The HYSYS basic rating model uses end-point calculations whereas the detailed model divides the heat exchanger in question into zones. The more zones, the more accurate the temperature profiles will be.

What makes the difference between end-point and weighted calculations important is that an end-point calculation uses the ΔT_{lm} for the exchanger to calculate the heat transfer rate using the standard heat transfer equation (equation 3.)

Table 9: Results of stepping the opening Z of VLV-103 from 10 to 95 %

Z (%)	ΔT_{cond} (°C)	F (kmol/s)	W_s (kJ/h)	P_h (kPa)
10	7,8	2,77	15 640	1 760
20	11,2	2,82	13 740	1 410
30	12,0	2,825	13 365	1 350
40	12,3	2,829	13 232	1 330
50	12,4	2,831	13 172	1 320
60	12,49	2,832	13 140	1 312
70	12,54	2,833	13 119	1 309
80	12,57	2,834	13 104	1 307
90	12,60	2,834	13 093	1 305
95	12,61	2,834	13 090	1 305

For this to be correct, the ΔT profile in the exchanger must be logarithmic (or flat). In an exchanger with phase change, the temperature profile will look more like the one shown in figure 48.

This means an end-point model will calculate a larger heat transfer than the weighted model, but it also means that the optimality of subcooling will not show.

The fact that the optimization simulations done with basic and detailed condenser model gave different results is an excellent illustration of the following: The level of detail in a process simulation should be considered carefully, based on what one wants to study. Although a simple model can be useful for studying large-scale dynamics and gives rough estimates on different process parameters, a precise optimization requires greater detail.

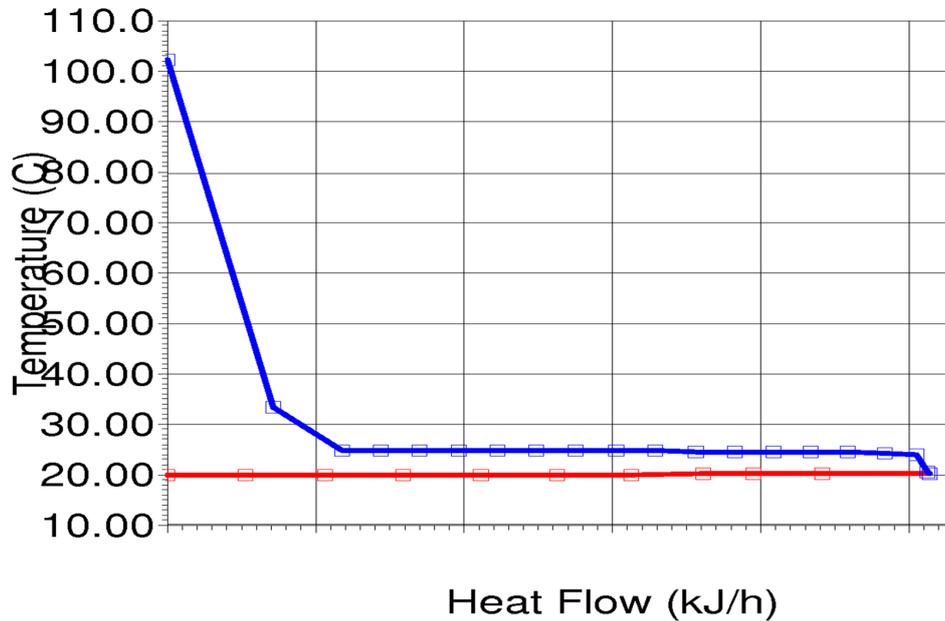
3.8.3 Controller tuning and operation

When considering what choice of controlled variable for the optimization DOF that would be the best for actual operation of the cycle, both disturbance rejection and set point tracking is important.

For the linear increase in T_h , controlling the subcooling was no doubt the best choice. Control of ΔT gave oscillation in the manipulated variable (could also be due to tuning, but considering that the same tuning rules were used for all three cases, this is not likely). Although controlling P_h gave smooth control up to a certain time, there was some oscillation in the last minutes before T_h was reset to the nominal value.

For the step in T_h down to 20°C, controlling the subcooling gave much smoother response than the other two cases.

For the series of steps in $Q_{c,s}$ controlling ΔT gave the smoothest response, but the input usage was actually smaller for the case with ΔT_{sub} control. For pressure control, the response was not as smooth as for control of ΔT and the manipulated variable went to saturation (and stayed there



zero. Actually, the same was observed at any time when the superheating was zero. The ‘trend’ of the variables is just as one would expect from the disturbance and the controller settings, but with the small spikes. Whether this is due to modelling errors or numerical errors is hard to tell, but it does not seem to affect the behaviour of the process on a longer time scale than half a minute.

The fact that the process seemed to stabilize with nonzero superheating, was probably because the low-pressure tank which the superheated stream entered (V-101) had a large holdup. With a large holdup one can have a sort of pseudo-steady state, where the streams entering and leaving the tank have slightly different conditions. This could make some variables change very slowly, and using very long time to reach steady state.

It would probably be wise to initialize V-101 with a lower liquid level - it should probably be so low that the tank could accomodate all the liquid in the other holdups in the cycle, but not lower than that all the other holdups could be completely full and V-101 not running empty.

3.9 Conclusions, ammonia cycle

From the simulations that have been carried out, the following conclusions can be made:

- It is optimal to maintain some subcooling in the liquid ammonia stream leaving the condenser. This optimality will not show if one uses an end-point model for rating of the condenser. This means the basic rating model for heat exchangers in HYSYS should not be used for studying processes where phase change takes place.
- For the simple ammonia cycle studied here, control of the condenser outlet ΔT and of the subcooling ΔT_{sub} are both working in practice - controlling the subcooling seems to give the best control.
- The SIMC rules for tuning of PID controllers give satisfying performance when the process is subject to the different disturbances considered here.

4 Case study: C3-MR Process

The C3-MR process is a natural gas liquefaction process where the natural gas is first pre-cooled with propane, and then cooled further with a mixture of light hydrocarbons (MR means Mixed Refrigerant). The used MR is regenerated by first compressing it and cooling with water, and then cooling it with propane, too. This means both MR and natural gas are cooled with propane. The process is described in [7] and in the report from the work done at Norsk Hydro in 2006 [10]. Numerical values are only approximate and may deviate from conditions in the actual process.

4.1 Process description

4.1.1 Processing of the natural gas

CO₂ and sulfur are removed from the natural gas, which is fed to the propane vaporizers. In the process considered here, there are three pressure levels, so there are three propane vaporizers for cooling natural gas. (There are also three for cooling the MR). When it leaves the last propane vaporizer at between -30°C and -40°C , it is fed to a fractionation column where components heavier than propane are removed from the mixture. The overhead stream from the column is condensed in the bottom bundle of the main cryogenic heat exchanger (from here abbreviated MCHE). This is a spiral-wound heat exchanger where the hot fluid flows upwards inside the tubes and cold fluid pours down outside the tubes. The partially condensed stream goes to the column's reflux drum. The vapour from the drum goes to the middle bundle of the MCHE, the liquid is refluxed to the column.

The natural gas mixture then travels through the middle and upper bundles of the MCHE. When it leaves on the top, it is subcooled at high pressure. It is flashed in a valve and enters a separator tank at -162°C and slightly above atmospheric pressure. The gas phase from the separator is heated by heat exchange with some of the mixed refrigerant, and used as fuel in the process. The liquid phase is pumped to LNG storage tanks.

4.1.2 Propane (C3) loop

For each pressure level there are two vaporizers: One for cooling natural gas, one for cooling the MR. This gives a total of six propane vaporizers. There are several possible setups for the propane loop:

- The propane stream can be split to the high-pressure vaporizers, and for each pressure level, the gas goes to the compressor and the liquid goes to the next pressure level.
- There may be one stream split before each exchanger, so that the propane entering each vaporizer is not larger than that all of it is

vaporized.

For both alternatives, the propane vapor leaving each vaporizer goes to the corresponding compressor stage. Thus the propane compressor has three stages. Before each vaporizer there is a choke valve that reduces pressure and temperature.

The propane loop may or may not contain liquid receivers. For safety reasons it will typically have a suction drum before each compressor, this is because the feed stream to a gas compressor should never contain liquid as this could damage the compressor. The process may also contain a liquid receiver after the condenser, on the high-pressure side.

4.1.3 Mixed Refrigerant (MR) loop

When the mixed refrigerant (abbreviated MR) leaves the MCHE it should be 100 % vapour. It is compressed from the low pressure at which it leaves the MCHE to a pressure well above 40 bar, in three compressor stages with water coolers between them. Then the high pressure MR is cooled with vaporizing propane to about the same temperature as the natural gas. It enters a gas-liquid separator tank. The liquid is fed to the bottom bundle of the MCHE and travels through the bottom and middle bundles. It leaves the middle bundle at about the same temperature as the natural gas leaving the same bundle, and is flashed to a lower pressure before entering the shell side of the MCHE.

The gas fraction from the MR gas-liquid separator is split in two streams. The larger stream enters the bottom bundle of the MCHE and travels through all three bundles of the exchanger, leaving on the top. It is then expanded in a valve and enters the shell side of the MCHE. The other stream is used to heat the fuel gas from the LNG separator tank, after the exchanger it is expanded in a valve and enters the shell side of the MCHE together with the other stream.

The MR pours down over the tube bundles of the MCHE, and leaves the bottom of the exchanger completely vaporized before entering the first compressor stage, closing the loop.

4.2 Control of C3-MR process

A simplified flow sheet is shown in figure 49. The fractionation column, the LNG flash tank used to reduce the nitrogen content and take off a fuel gas stream, and the fuel gas heater are omitted.

The main goals of control are to deliver an maximal flow of liquefied natural gas (LNG) at the correct pressure and with a content of N_2 below a specific limit, and to maintain safe operating conditions in all process units. Safe operation means to stay within certain constraints, among these are:

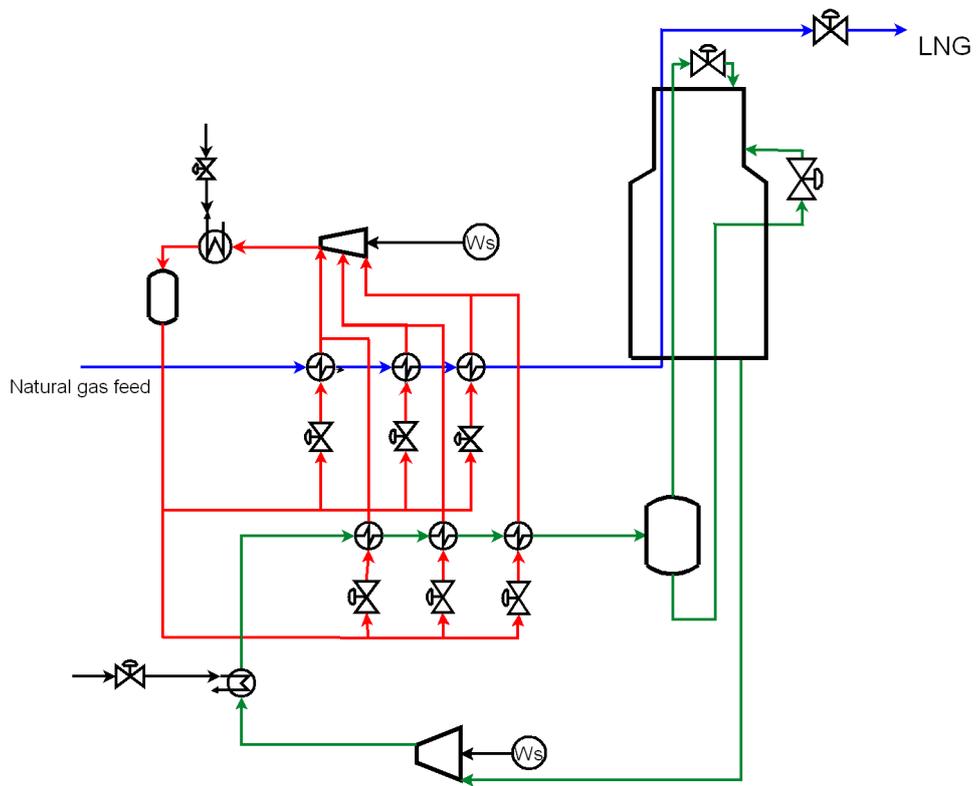


Figure 49: Simplified flow sheet of the C3MR process

- The feed to the compressors must be exclusively vapour. Any liquid present may damage the compressors.
- Pressures should be kept within given limits given by the specifications of the process equipment.
- No streams should be allowed to freeze - it might damage the process equipment or plug tubes, reducing the throughput.

4.2.1 Degree of freedom analysis

The variables that can be physically manipulated in the process are:

- The opening of the six choke valves in the propane precooling cycle
- The propane compressor speed
- The MR compressor speed
- The flow of cooling water in the two water coolers (the propane condenser and the MR water cooler after the compressor)
- The opening of the two J-T-valves in the MR cycle
- The opening of the LNG J-T valve

This gives a total of 13 manipulated inputs. Some of these will have to be used to stabilize levels and some will need to control active constraints:

- The levels in the propane vaporizers need to be controlled, to avoid liquid in the compressors or the vaporizers running empty. This consumes six control degrees of freedom.
- The temperature of the natural gas stream at the MCHE outlet must be controlled at its constraint (cooling below the specified maximum temperature is possible, but uneconomical). This consumes one degree of freedom.
- The cooling water flows may (and will often) be set to maximum as cooling water is cheap compared to compression work. This means two manipulated variables are at their constraint value. Two further degrees of freedom are consumed.

As we can see, a total of 9 degrees of freedom are used to stabilize levels and control the active constraints. This means four manipulated variables can be used to either maximize the throughput of natural gas using the maximum available compressor power, or to minimize the compressor power consumption for a given flow of natural gas.

4.2.2 Choice of controlled variables

The choke valves in the propane loop can be used to stabilize the levels in the vaporizers. This would be practical as the inputs and outputs are physically close to each other, so that any delay would be small.

With the sea water flows fixed at maximum, there are five manipulated inputs left to use for control. One of these must control the temperature of the natural gas stream at the outlet of the MCHE as this is an active constraint in the process. For this one may, for example, use the LNG expansion valve.

The remaining four variables should be used to either maximize the flow rate of natural gas using the maximal available compressor power, or to minimize the compressor power for a given flow. If the LNG expansion valve is used to control the NG temperature at the MCHE outlet, these variables are the speeds of the MR and propane compressors and the opening of the two MR choke valves.

- For the case when one wants to maximize the flow, the compressors will both run at maximum speed. One of the two choke valves will be setting the flow of LNG and the other will be used to maximize the compressor power used. The set point of the flow controller is increased until both compressors are at their peak power.
- For the case when natural gas flow is given, one of the choke valves is used to set this flow. With the two compressors controlling one variable each, the last choke valve will be used to minimize the power consumption.

With the above in mind, which variables the compressors should control and which ones should be controlled by the choke valves? One of the choke valves would have to be used to set the throughput of natural gas. The compressors can control the temperatures of natural gas and MR to the MCHE. The last choke valve, which is used to optimize the operation, should ideally control a self-optimizing variable. There are many possible variables - one can control temperature differences, pressures, or the active charge in the MR cycle. Controlling the active charge in the MR cycle would correspond to controlling the liquid level in the MR flash tank. To find the best choice of controlled variable, one would first find the optimal values of the process variables for each case (max production and given flow). Then one would introduce disturbances to the model to find the changes in optimal values for the different candidate variables as it is, for example, carried out in the study on the PRICO process done by Jensen/Skogestad [11].

4.3 Modelling the process in HYSYS

In order to try out control structures for the process, a dynamic model was built in Aspen HYSYS 2004.2. The following simplifications were made:

- The fractionation column was omitted. This meant that the lower and middle parts of the MCHE could be merged into one part
- The MCHE was replaced by shell-and-tube heat exchangers where the cold refrigerant stream was divided in two (upper part of MCHE) and three (lower and middle parts)

In the model, the MR side stream used to heat the fuel gas stream was included. This does not give or consume any degrees of freedom as there is a choke valve on the side stream as well, and this choke valve can be used to control the fuel gas temperature. The LNG flash tank is an additional level that needs to be controlled, but this is done by the pump at the liquid outlet of the tank. Thus there is no change in the number of DOFs for optimizing operation.

There was not sufficient time to complete the model with the desirable level of detail. Most heat exchangers were initially modelled with the basic rating model to find approximate UA values. (For the exchangers resembling the MCHE, the detailed model was used). For a detailed study, one should use the detailed rating model for all exchangers, at least for the exchangers where phase change takes place. In addition, one should specify that the vapour outlet nozzles of the propane vaporizers are located on top of the exchangers, to assure liquid does not enter the compressors. This requires use of the ‘Fidelity’ option in HYSYS and also requires that the detailed model is used for the exchangers in question.

As HYSYS 2004.2 does not accommodate multistage compressor models, the propane compressor is modelled as three separate compressors. To bring the realism to the maximal, these will need to be linked so they operate at the same speed. To be able to study the case of maximizing LNG production for maximal compressor speed, one should try to supply as realistic compressor curves as possible as well.

The MR compressor, which has three stages with intercooling, is also modelled as three separate compressors, with heat exchangers between them and a final heat exchanger after the third compressor. The three compressors should be linked so they run at the same speed, just as for the propane compressor.

For the LNG pump, one must also supply a curve, but the accuracy of this curve is not as crucial as for the compressors, as pump work here is negligible compared to the work of compressing propane and MR.

Flow sheets and process data are shown in appendix A.

4.4 Conclusions and further work, C3MR process

For both the case of given flow and the case of maximum compressor power usage, there is one degree of freedom available for optimization of the process.

Further work on the process can include the following:

- Finding accurate compressor curves and heat exchanger rating data
- Steady state optimization
- To identify candidates for controlled variables for the last manipulated variable
- To examine which ones of these variables that are suited to give self-optimizing control of the process

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- [11] Jensen, Jørgen B., Skogestad, S.: Optimal operation of a simple LNG process, *Adchem* 2006

Nomenclature

$(\frac{dm}{dt})_{scaled}$	Rate of change in % of maximum holdup
ΔP	Pressure drop in process unit
ΔQ_c	Change in Q_c in % of range
ΔT	Temperature difference at condenser outlet
ΔT_{lm}	Mean logarithmic temperature difference
ΔT_{sub}	Subcooling at condenser outlet
ΔW_s	Change in W_s in % of range
ΔZ	Change in valve opening
$\frac{dm}{dt}$	Rate of change in holdup
μ	Efficiency of cycle
ρ	Density of fluid
τ	Time constant in transfer function
τ_c	Tuning parameter in SIMC tuning rules
τ_D	Derivative time of PID controller
τ_I	Integral time of PI(D) controller
θ	Delay
A	Heat transfer area in exchanger
C_V, C_g	Constants in valve equations
COP	Coefficient of performance
COP_{Carnot}	Coefficient of performance of ideal Carnot cycle
f	Flow rate
f_t	Exchanger geometry correction factor
$g(s)$	Transfer function
k	In transfer functions: Steady state gain
k	Pressure-flow relation constant
K_c	Proportional gain of controller

Q	Heat transferred in exchanger
Q_c	Heat removed from cold reservoir at T_C
$Q_{c,s}$	Set point for heat transferred at T_c
s	Laplace variable
T_c	Temperature of cold reservoir
T_h	Temperature of hot reservoir
T_{sat,P_h}	Boiling point at pressure P_h
U	Overall heat transfer coefficient
W_s	Compressor shaft work
Z	Opening of valve in %

List of attached files

The following computer files are attached:

1. Ammonia cycle dyn optim.hsc: Contains the optimization sequence
2. Ammonia cycle, tuning of controllers.hsc: The case with tuning of controllers (except the pressure controller)
3. Ammonia cycle, tuning of PIC.hsc: Tuning of the pressure controller
4. Ammonia cycle, regtest case I.hsc: Control testing case I
5. Ammonia cycle. regtest case II.hsc: Control testing case II
6. Ammonia cycle, regtest case III.hsc: Control testing case III
7. C3MR, dynamic model.hsc: Dynamic model of C3MR process (initial, ready to run)
8. diplom.pdf: Electronic copy of this thesis

A HYSYS model of C3-MR process

A.1 Flow sheets of HYSYS model

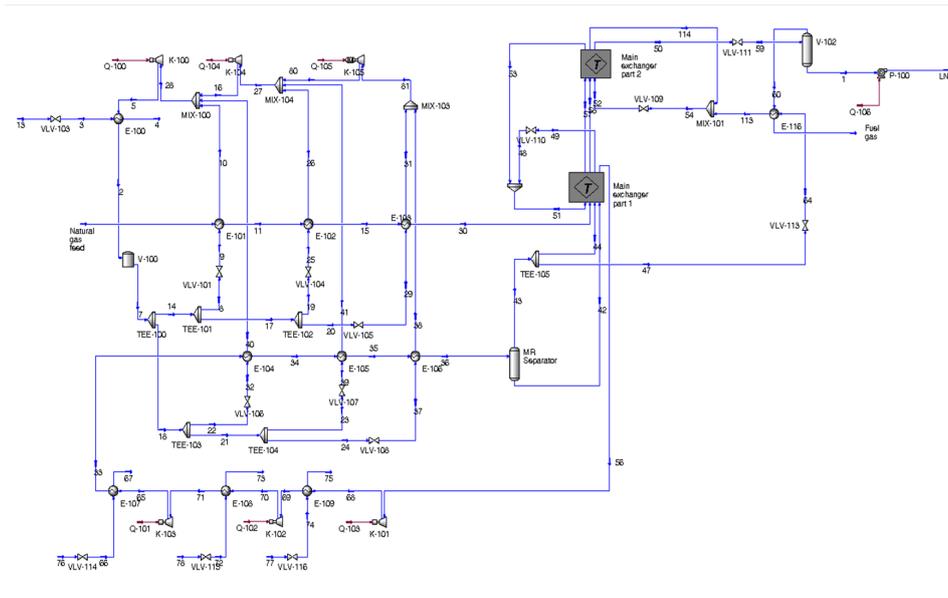


Figure 50: Entire flow sheet of HYSYS model of C3-MR process. Controllers and spread sheets not shown

Figure 50 shows the HYSYS flow sheet. The two boxes marked ‘T’ are the sub-flowsheets that correspond to the upper and lower parts of the main cryogenic heat exchanger (MCHE).

Figure 51 shows the propane loop blown up to see this part of the process in better detail.

Figure 52 shows how MR leaving the bottom of the MCHE is regenerated (compressed and cooled).

Figure 53 shows the part of the process where the natural gas is liquefied and the fuel gas stream is taken off and heated. Notice the two sub-flowsheets labeled ‘Main exchanger part 1’ and ‘Main exchanger part 2’.

Figure 54 shows the sub-flowsheet that resembles the middle and lower bundles of the main cryogenic heat exchanger. The cold MR (stream 51) enters, is split in three streams and is used to cool MR vapour (stream 44), MR liquid (42) and natural gas (stream 30).

Figure 55 shows the sub-flowsheet that resembles the upper bundle of the main cryogenic heat exchanger. The cold MR (stream 52) enters, is split

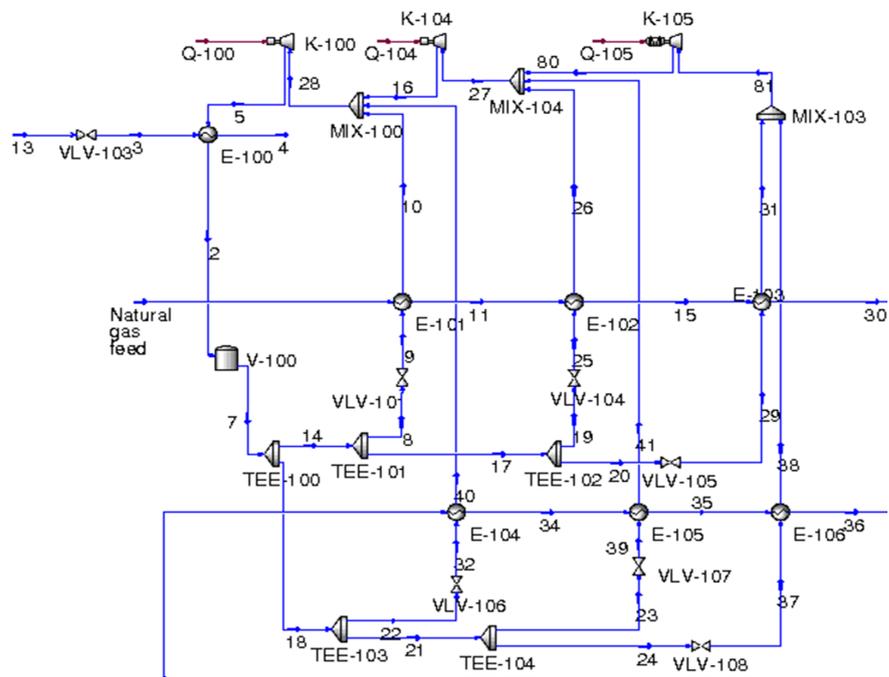


Figure 51: HYSYS flow sheet of propane loop in C3-MR process

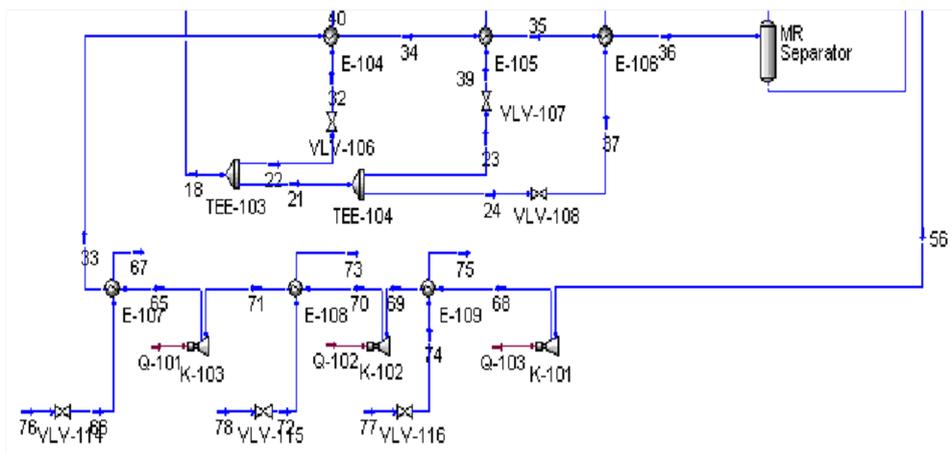


Figure 52: HYSYS flow sheet of MR regeneration

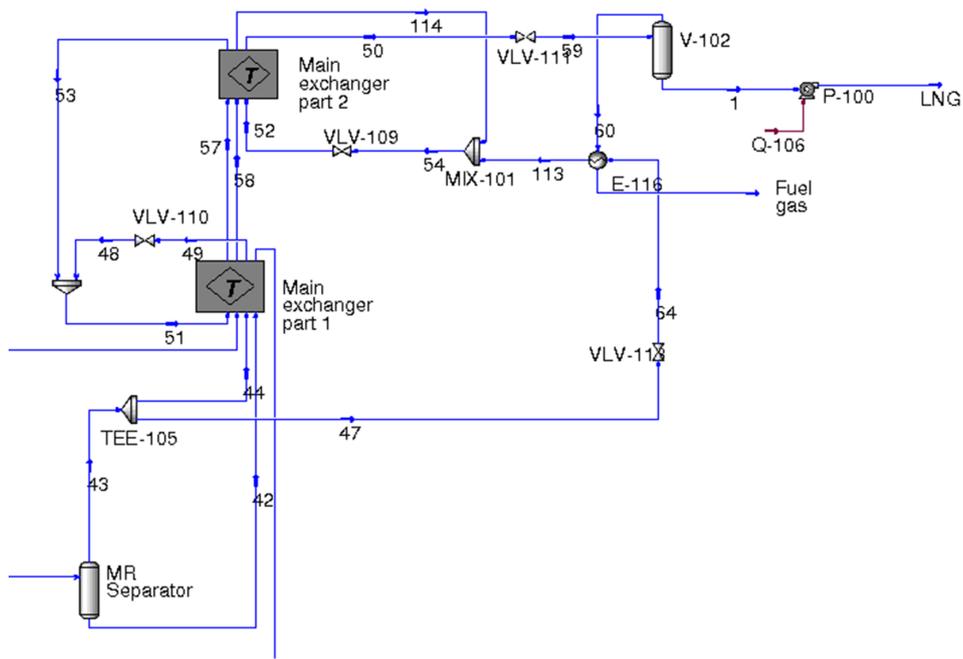


Figure 53: MR flash, MCHE, LNG flash, fuel gas recovery

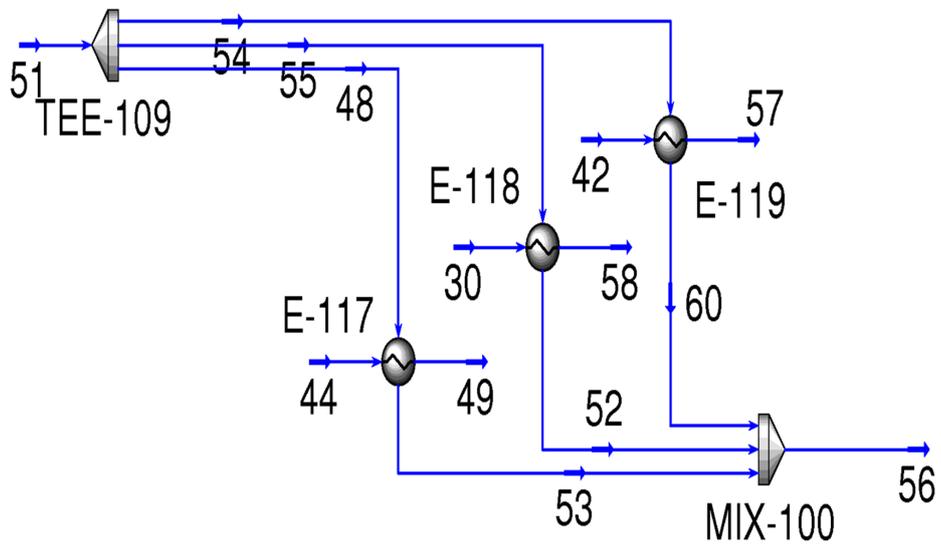


Figure 54: Sub-flowsheet for the lower part of the MCHE

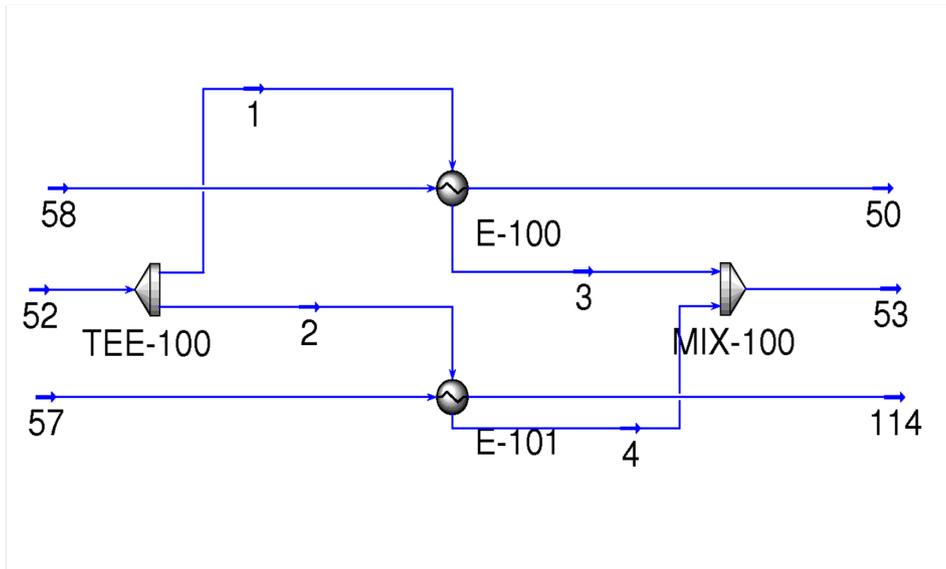


Figure 55: Sub-flowsheet for the lower part of the MCHE

in two streams and is used to cool the hotter MR (stream 57) and natural gas (stream 58).

A.2 HYSYS stream data

The tables in this subsection are printed directly from the HYSYS case. The stream numbers refer to the flow sheets shown in A.1. For the 'MCHE part 1' and 'MCHE part 2' the stream numbers refer to the respective subflowsheets.

Workbook: Main exchanger part 1 (TPL1)							
Material Streams						Fluid Pkg: All	
Name	48	54	55	44	49		
Vapour Fraction	0.5950	0.5950	0.5950	1.0000	0.3755		
Temperature (C)	-104.7	-104.7	-104.7	-38.00	-81.68		
Pressure (kPa)	173.3	173.3	173.3	4570	3800		
Molar Flow (kgmole/h)	1330	2027	4043	2073	2073		
Mass Flow (kg/h)	3.239e+004	4.937e+004	9.847e+004	4.273e+004	4.273e+004		
Liquid Volume Flow(m3/h)	90.77	138.3	275.9	121.0	121.0		
Heat Flow (kJ/h)	-1.179e+008	-1.796e+008	-3.583e+008	-1.516e+008	-1.632e+008		
Name	53	51	30	58	52		
Vapour Fraction	1.0000	0.5950	1.0000	0.0323	1.0000		
Temperature (C)	-40.47	-104.7	-36.62	-85.72	-43.00		
Pressure (kPa)	153.3	173.3	4440	3670	153.3		
Molar Flow (kgmole/h)	1330	7400	5000	5000	4043		
Mass Flow (kg/h)	3.239e+004	1.802e+005	9.263e+004	9.263e+004	9.847e+004		
Liquid Volume Flow(m3/h)	90.77	505.0	286.5	286.5	275.9		
Heat Flow (kJ/h)	-1.063e+008	-6.558e+008	-3.963e+008	-4.311e+008	-3.235e+008		
Name	42	57	60	56			
Vapour Fraction	0.0000	0.0000	1.0000	1.0000			
Temperature (C)	-38.00	-81.67	-40.21	-41.78			
Pressure (kPa)	4570	3800	153.3	153.3			
Molar Flow (kgmole/h)	5127	5127	2027	7400			
Mass Flow (kg/h)	1.334e+005	1.334e+005	4.937e+004	1.802e+005			
Liquid Volume Flow(m3/h)	372.4	372.4	138.3	505.0			
Heat Flow (kJ/h)	-4.793e+008	-4.969e+008	-1.620e+008	-5.917e+008			

Figure 56: Stream data for streams in MCHE part 1 flow sheet

Workbook: Case (Main)

	Streams					Fluid Pkg: All
	7	8	9	10	11	
11 Name						
12 Vapour Fraction	0.0000	0.0000	0.1403	0.9820	1.0000	
13 Temperature (C)	20.00	20.00	9.761e-004	-6.846e-002	1.675	
14 Pressure (kPa)	836.2	836.2	473.5	472.5	4460	
15 Molar Flow (kgmole/h)	5604	314.0	314.0	314.0	5000	
16 Mass Flow (kg/h)	2.471e+005	1.385e+004	1.385e+004	1.385e+004	9.263e+004	
17 Std Ideal Liq Vol Flow (m3/h)	487.7	27.33	27.33	27.33	286.5	
18 Heat Flow (kJ/h)	-6.761e+008	-3.788e+007	-3.788e+007	-3.349e+007	-3.868e+008	
19 Molar Enthalpy (kJ/kgmole)	-1.207e+005	-1.207e+005	-1.207e+005	-1.067e+005	-7.736e+004	
20 Name	Natural gas feed	13	14	16	17	
21 Vapour Fraction	1.0000	0.0000	0.0000	1.0000	0.0000	
22 Temperature (C)	20.84	9.995*	20.00	14.84	20.00	
23 Pressure (kPa)	4470*	131.7*	836.2	472.5	836.2	
24 Molar Flow (kgmole/h)	5000	1.212e+005	1062	4653	748.0	
25 Mass Flow (kg/h)	9.263e+004	2.184e+006	4.683e+004	2.052e+005	3.298e+004	
26 Std Ideal Liq Vol Flow (m3/h)	286.5	2188	92.43	405.0	65.10	
27 Heat Flow (kJ/h)	-3.824e+008	-3.484e+010	-1.281e+008	-4.896e+008	-9.025e+007	
28 Molar Enthalpy (kJ/kgmole)	-7.648e+004*	-2.874e+005	-1.207e+005	-1.052e+005	-1.207e+005	
29 Name	18	19	20	21	22	
30 Vapour Fraction	0.0000	0.0000	0.0000	0.0000	0.0000	
31 Temperature (C)	20.00	20.00	20.00	20.00	20.00	
32 Pressure (kPa)	836.2	836.2	836.2	836.2	836.2	
33 Molar Flow (kgmole/h)	4542	360.0	388.0	3905	637.0	
34 Mass Flow (kg/h)	2.003e+005	1.587e+004	1.711e+004	1.722e+005	2.809e+004	
35 Std Ideal Liq Vol Flow (m3/h)	395.3	31.33	33.77	339.9	55.44	
36 Heat Flow (kJ/h)	-5.480e+008	-4.343e+007	-4.681e+007	-4.711e+008	-7.686e+007	
37 Molar Enthalpy (kJ/kgmole)	-1.207e+005	-1.207e+005	-1.207e+005	-1.207e+005	-1.207e+005	
38 Name	23	24	25	26	28	
39 Vapour Fraction	0.0000	0.0000	0.2533	0.9947	1.0000	
40 Temperature (C)	20.00	20.00	-20.00	-20.12	11.16	
41 Pressure (kPa)	836.2	836.2	244.2	243.2	472.5	
42 Molar Flow (kgmole/h)	2050	1855	360.0	360.0	5604	
43 Mass Flow (kg/h)	9.040e+004	8.180e+004	1.587e+004	1.587e+004	2.471e+005	
44 Std Ideal Liq Vol Flow (m3/h)	178.4	161.4	31.33	31.33	487.7	
45 Heat Flow (kJ/h)	-2.473e+008	-2.238e+008	-4.343e+007	-3.871e+007	-5.913e+008	
46 Molar Enthalpy (kJ/kgmole)	-1.207e+005	-1.207e+005	-1.207e+005	-1.075e+005	-1.055e+005	
47 Name	29	30	31	32	33	
48 Vapour Fraction	0.3399	1.0000	1.0000	0.1403	1.0000	
49 Temperature (C)	-38.00	-36.62	-37.77	0.0000	19.99	
50 Pressure (kPa)	121.3	4440	120.3	473.5	4600	
51 Molar Flow (kgmole/h)	388.0	5000	388.0	637.0	7400	
52 Mass Flow (kg/h)	1.711e+004	9.263e+004	1.711e+004	2.809e+004	1.802e+005	
53 Std Ideal Liq Vol Flow (m3/h)	33.77	286.5	33.77	55.44	505.0	
54 Heat Flow (kJ/h)	-4.681e+007	-3.963e+008	-4.206e+007	-7.686e+007	-5.865e+008	
55 Molar Enthalpy (kJ/kgmole)	-1.207e+005	-7.926e+004	-1.084e+005	-1.207e+005	-7.925e+004	
56 Name	34	36	37	38	39	
57 Vapour Fraction	1.0000	0.3178	0.3399	1.0000	0.2533	
58 Temperature (C)	2.011	-37.26	-38.00	-37.54	-20.00	
59 Pressure (kPa)	4590	4570	121.3	120.3	244.2	
60 Molar Flow (kgmole/h)	7400	7400	1855	1855	2050	
61 Mass Flow (kg/h)	1.802e+005	1.802e+005	8.180e+004	8.180e+004	9.040e+004	
62 Std Ideal Liq Vol Flow (m3/h)	505.0	505.0	161.4	161.4	178.4	
63 Heat Flow (kJ/h)	-5.952e+008	-6.447e+008	-2.238e+008	-2.011e+008	-2.473e+008	
64 Molar Enthalpy (kJ/kgmole)	-8.043e+004	-8.712e+004	-1.207e+005	-1.084e+005	-1.207e+005	



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Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

	40	41	42	43	44
Name					
Vapour Fraction	0.9612	0.9916	0.0000	1.0000	1.0000
Temperature (C)	-6.836e-002	-20.11	-38.00	-38.00	-38.00
Pressure (kPa)	472.5	243.2	4570	4570	4570
Molar Flow (kgmole/h)	637.0	2050	5127	2273	2073
Mass Flow (kg/h)	2.809e+004	9.040e+004	1.334e+005	4.685e+004	4.273e+004
Std Ideal Liq Vol Flow(m3/h)	55.44	178.4	372.4	132.7	121.0
Heat Flow (kJ/h)	-6.816e+007	-2.205e+008	-4.793e+008	-1.662e+008	-1.516e+008
Molar Enthalpy(kJ/kgmole)	-1.070e+005	-1.076e+005	-9.348e+004	-7.313e+004	-7.313e+004
Name			Fuel gas		
Vapour Fraction	1.0000	0.0000	1.0000	0.1231	1.0000
Temperature (C)	-38.00	-146.4	-52.35	-162.0	-162.0
Pressure (kPa)	4570	3020	96.57 *	97.57	97.57
Molar Flow (kgmole/h)	200.0	5000	615.5	5000	615.5
Mass Flow (kg/h)	4122	9.263e+004	1.085e+004	9.263e+004	1.085e+004
Std Ideal Liq Vol Flow(m3/h)	11.67	286.5	31.44	286.5	31.44
Heat Flow (kJ/h)	-1.463e+007	-4.521e+008	-4.161e+007	-4.521e+008	-4.383e+007
Molar Enthalpy(kJ/kgmole)	-7.313e+004	-9.041e+004	-6.761e+004	-9.041e+004	-7.122e+004
Name					
Vapour Fraction	0.0000	0.9949	1.0000	0.0000	0.0000
Temperature (C)	-162.0	-39.00	70.04	10.01	18.46
Pressure (kPa)	97.57	4402	4610	106.7	105.7 *
Molar Flow (kgmole/h)	4385	200.0	7400	3.300e+004	3.300e+004
Mass Flow (kg/h)	8.178e+004	4122	1.802e+005	5.945e+005	5.945e+005
Std Ideal Liq Vol Flow(m3/h)	255.1	11.67	505.0	595.7	595.7
Heat Flow (kJ/h)	-4.082e+008	-1.463e+007	-5.648e+008	-9.484e+009	-9.462e+009
Molar Enthalpy(kJ/kgmole)	-9.311e+004	-7.313e+004	-7.632e+004	-2.874e+005	-2.867e+005
Name					
Vapour Fraction	1.0000	1.0000	0.0000	0.0000	0.0000
Temperature (C)	92.26	21.03	10.01	18.86	10.00 *
Pressure (kPa)	2500	2490	106.7	105.7 *	131.7 *
Molar Flow (kgmole/h)	7400	7400	4.000e+004	4.000e+004	3.300e+004
Mass Flow (kg/h)	1.802e+005	1.802e+005	7.206e+005	7.206e+005	5.945e+005
Std Ideal Liq Vol Flow(m3/h)	505.0	505.0	722.1	722.1	595.7
Heat Flow (kJ/h)	-5.511e+008	-5.787e+008	-1.150e+010	-1.147e+010	-9.484e+009
Molar Enthalpy(kJ/kgmole)	-7.448e+004	-7.820e+004	-2.874e+005	-2.867e+005	-2.874e+005
Name					
Vapour Fraction	0.0000	0.0000	1.0000	1.0000	1.0000
Temperature (C)	10.00 *	10.00 *	-18.18	-14.83	-7.093
Pressure (kPa)	131.7 *	131.7 *	4450	243.2	243.2
Molar Flow (kgmole/h)	4.500e+004	4.000e+004	5000	4653	2243
Mass Flow (kg/h)	8.107e+005	7.206e+005	9.263e+004	2.052e+005	9.891e+004
Std Ideal Liq Vol Flow(m3/h)	812.3	722.1	286.5	405.0	195.2
Heat Flow (kJ/h)	-1.293e+010	-1.150e+010	-3.915e+008	-4.982e+008	-2.389e+008
Molar Enthalpy(kJ/kgmole)	-2.874e+005	-2.874e+005	-7.831e+004	-1.071e+005	-1.065e+005
Name					
Vapour Fraction	1.0000	0.0000	0.0000	0.0000	1.0000
Temperature (C)	-37.58	20.00	10.00	20.00	38.44
Pressure (kPa)	120.3	836.2	106.7	96.72 *	837.2
Molar Flow (kgmole/h)	2243	5604	1.212e+005	1.212e+005	5604
Mass Flow (kg/h)	9.891e+004	2.471e+005	2.184e+006	2.184e+006	2.471e+005
Std Ideal Liq Vol Flow(m3/h)	195.2	487.7	2188	2188	487.7
Heat Flow (kJ/h)	-2.431e+008	-6.761e+008	-3.484e+010	-3.474e+010	-5.819e+008
Molar Enthalpy(kJ/kgmole)	-1.084e+005	-1.207e+005	-2.874e+005	-2.866e+005	-1.038e+005



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Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

	68	69	74	75	35
11 Name					
12 Vapour Fraction	1.0000	1.0000	0.0000	0.0000	0.6303
13 Temperature (C)	94.99	19.58	10.01	17.87	-18.12
14 Pressure (kPa)	1000	990.0	106.7	105.7*	4580
15 Molar Flow (kgmole/h)	7400	7400	4.500e+004	4.500e+004	7400
16 Mass Flow (kg/h)	1.802e+005	1.802e+005	8.107e+005	8.107e+005	1.802e+005
17 Std Ideal Liq Vol Flow (m3/h)	505.0	505.0	812.3	812.3	505.0
18 Heat Flow (kJ/h)	-5.471e+008	-5.746e+008	-1.293e+010	-1.290e+010	-6.220e+008
19 Molar Enthalpy (kJ/kgmole)	-7.393e+004	-7.765e+004	-2.874e+005	-2.868e+005	-8.405e+004
20 Name	113	49	53	56	57
21 Vapour Fraction	0.0000	0.3755	0.5447	1.0000	0.0000
22 Temperature (C)	-146.3	-81.68	-97.05	-41.78	-81.67
23 Pressure (kPa)	4392	3800	173.3	153.3	3800
24 Molar Flow (kgmole/h)	200.0	2073	5327	7400	5127
25 Mass Flow (kg/h)	4122	4.273e+004	1.375e+005	1.802e+005	1.334e+005
26 Std Ideal Liq Vol Flow (m3/h)	11.67	121.0	384.0	505.0	372.4
27 Heat Flow (kJ/h)	-1.685e+007	-1.632e+008	-4.929e+008	-5.917e+008	-4.969e+008
28 Molar Enthalpy (kJ/kgmole)	-8.425e+004	-7.872e+004	-9.252e+004	-7.996e+004	-9.693e+004
29 Name	58	114	48	51	52
30 Vapour Fraction	0.0323	0.0000	0.5967	0.5950	0.0341
31 Temperature (C)	-85.72	-148.8	-112.2	-104.7	-150.5
32 Pressure (kPa)	3670	3500	1000	173.3	183.3
33 Molar Flow (kgmole/h)	5000	5127	2073	7400	5327
34 Mass Flow (kg/h)	9.263e+004	1.334e+005	4.273e+004	1.802e+005	1.375e+005
35 Std Ideal Liq Vol Flow (m3/h)	286.5	372.4	121.0	505.0	384.0
36 Heat Flow (kJ/h)	-4.311e+008	-5.190e+008	-1.632e+008	-6.558e+008	-5.359e+008
37 Molar Enthalpy (kJ/kgmole)	-8.622e+004	-1.012e+005	-7.872e+004	-8.862e+004	-1.006e+005
38 Name	54	LNG			
39 Vapour Fraction	0.0000	0.0000			
40 Temperature (C)	-148.7	-162.0			
41 Pressure (kPa)	3500	101.3*			
42 Molar Flow (kgmole/h)	5327	4385			
43 Mass Flow (kg/h)	1.375e+005	8.178e+004			
44 Std Ideal Liq Vol Flow (m3/h)	384.0	255.1			
45 Heat Flow (kJ/h)	-5.359e+008	-4.082e+008			
46 Molar Enthalpy (kJ/kgmole)	-1.006e+005	-9.311e+004			

A.3 Heat exchanger data

The UA values and pressure drops for the heat exchangers are shown in tables 10, 11 and 12.

Workbook: Main exchanger part 2 (TPL2)								
Material Streams							Fluid Pkg:	All
11	Name	1	2	3	4	58		
12	Vapour Fraction	0.0341	0.0341	0.5440	0.5454	0.0323		
13	Temperature (C)	-150.5	-150.5	-97.09	-97.01	-85.72		
14	Pressure (kPa)	183.3	183.3	173.3	173.3	3670		
15	Molar Flow (kgmole/h)	2600	2727	2600	2727	5000		
16	Mass Flow (kg/h)	6.712e+004	7.040e+004	6.712e+004	7.040e+004	9.263e+004		
17	Liquid Volume Flow(m3/h)	187.4	196.6	187.4	196.6	286.5		
18	Heat Flow (kJ/h)	-2.616e+008	-2.744e+008	-2.406e+008	-2.523e+008	-4.311e+008		
19	Name	53	52	50	57	114		
20	Vapour Fraction	0.5447	0.0341	0.0000	0.0000	0.0000		
21	Temperature (C)	-97.05	-150.5	-146.4	-81.67	-148.8		
22	Pressure (kPa)	173.3	183.3	3020	3800	3500		
23	Molar Flow (kgmole/h)	5327	5327	5000	5127	5127		
24	Mass Flow (kg/h)	1.375e+005	1.375e+005	9.263e+004	1.334e+005	1.334e+005		
25	Liquid Volume Flow(m3/h)	384.0	384.0	286.5	372.4	372.4		
26	Heat Flow (kJ/h)	-4.929e+008	-5.359e+008	-4.521e+008	-4.969e+008	-5.190e+008		

Figure 57: Stream data for streams in MCHE part2 flow sheet

Table 10: UA values and pressure drops for heat exchangers in HYSYS model, main flow sheet

Exchanger	Shell ΔP	Tube ΔP	UA
E-100	1,0 kPa	10,0 kPa	$2,376 \cdot 10^7 \frac{kJ}{K \cdot hour}$
E-101	1,0 kPa	10,0 kPa	$4,100 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-102	1,0 kPa	10,0 kPa	$4,100 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-103	1,0 kPa	10,0 kPa	$4,540 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-104	1,0 kPa	10,0 kPa	$7,900 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-105	1,0 kPa	10,0 kPa	$2,240 \cdot 10^6 \frac{kJ}{K \cdot hour}$
E-106	1,0 kPa	10,0 kPa	$2,250 \cdot 10^6 \frac{kJ}{K \cdot hour}$
E-107	1,0 kPa	10,0 kPa	$8,550 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-108	1,0 kPa	10,0 kPa	$7,750 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-109	1,0 kPa	10,0 kPa	$7,400 \cdot 10^5 \frac{kJ}{K \cdot hour}$
E-116	1,0 kPa	10,0 kPa	$1,534 \cdot 10^5 \frac{kJ}{K \cdot hour}$

A.4 Other model specifications

The Peng-Robinson equation of state was used for thermodynamic calculations. The compositions of the different streams are summarized in table 13.

For all compressors the nominal polytropic efficiency was set to 75 %.

Table 11: UA values and pressure drops for heat exchangers in HYSYS model, MCHE part 1 subflowsheet

Exchanger	Shell ΔP	Tube ΔP	UA
E-117	20,0 kPa	770,0 kPa	$1,259 \cdot 10^6 \frac{kJ}{K \cdot hour}$
E-118	20,0 kPa	770,0 kPa	$3,005 \cdot 10^6 \frac{kJ}{K \cdot hour}$
E-119	20,0 kPa	770,0 kPa	$1,990 \cdot 10^6 \frac{kJ}{K \cdot hour}$

Table 12: UA values and pressure drops for heat exchangers in HYSYS model, MCHE part 2 subflowsheet

Exchanger	Shell ΔP	Tube ΔP	UA
E-100	10,0 kPa	650,0 kPa	$2,945 \cdot 10^6 \frac{kJ}{K \cdot hour}$
E-101	10,0 kPa	300,0 kPa	$3,565 \cdot 10^6 \frac{kJ}{K \cdot hour}$

Table 13: Composition of streams - mole fractions of the different components

Stream	Methane	Ethane	Propane	Nitrogen
NG feed	0.85	0.10	0.03	0.02
Propane refrigerant	0	0	1	0
Mixed refrigerant	0.45	0.45	0.05	0.05