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Modeling and optimization of the methane extraction unit in T100/T200 at Kårstø

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Abstract

A model for the demethanizer in train T100/T200 at Kårstø was developed in Unisim. The model showed reasonable correlation with plant data and the existing model in D-spice for approximate Åsgard feed at high rate. An optimization was carried out for Åsgard feed at high rate, to a cost function found by market data. The controlled variables in the plant was used at degree of freedom. Two active constraint were found. The pressure before expansion has its optimal value at the boundary of 78 bar , and the column bottom temperature has its optimal when the temperature at tray 19 is kept at $-30 \text{ }^\circ\text{C}$. The temperature before the feed separator is found to be kept as low as possible. An internal minimum was found for the split of liquid from the cold separator. It was found that the optimal was to send 33% of the flow directly to the top of the column.

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1 Introduction

Gas from the North sea has become a valuable resource in our the modern word. It is for example used for cooking, heating and as a raw material in chemical synthesis. In nearly every store you can find plastic products originating from gas hydrocarbons. The gas arriving from the north sea is consisting of many components. Methane, ethane, propane, butane and traces of heavier components. It is the ethane and heavier components, called liquid components, that has it most valuable.

Kårstø is gas processing plant located in Tysvær north of Stavanger. Gas is arriving by pipeline from the north sea. At Kårstø the gas is fractionated in to its components to increase its value. The fractionation is done by distillation. Methane is first separated out from heavier components in the distillation column called the demethanizer. The methane is compressed and sent to the continent trough pipelines.

The two identical fractionation trains T100 and T200 has been in operation since the first gas arrived at Kårstø in 1985 [1]. The goal of the project is to get better understanding of how the set point in the demethanizer in T100/T200 effects the profit of the plant. The cost of operation the the plant is to be minimized while maximizing the income. The study is done by building a model of the demethanizer in UniSim and systematically changing the specifications corresponding to the controllers of the real plant. The optimal goal is to find the global minimum of the cost function.

The report is built up in three part. The process is first described following the derivation of the Model in UniSim. In the second part, the derived model is compared to the existing model in D-spice and plant data, to validate the quality of the model. Finally a cost function for the demethanizer is derived and the model is studied with respect to the cost function.

2 Process description

Kårstø is a gas fractionation facility located on the west coast of Norway. Gas enters from the north sea trough the pipelines Statpipe, Sleipner and Åsgard. Statpipe is fractionated in the the two identical trains, train T100 and train T200. The gas goes trough several filters and a drying sequence before arriving at the demethanizer. In the demethanizer the methane is separated out by distillation. The gas enters the section at approximately 110 bar, has a temperature of 5° C and contains 85 mol% methane. A simplified flow diagram for the section is presented in figure 2.1.

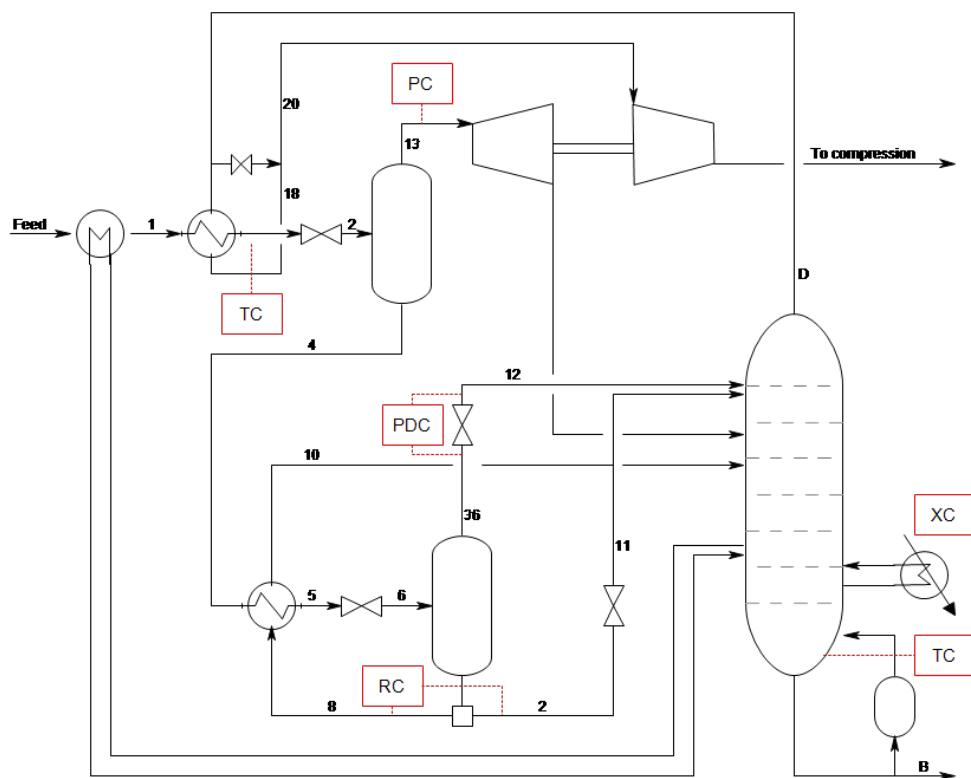


Figure 2.1: Flow diagram for the demethaniser section

The entering gas to the section is precooled by a side flow from the column and the column distillate. The temperature after cooler is controlled by bypassing parts of the distillate flow. It is favorable to have the temperature as low as possible both for the feed and distillate flow after the heat exchanger. Lower temperature in the distillate reducing the work needed in the subsequent compression, and lower temperature in the feed reduces the temperature in the cold

separator (first flash tank).

To reduce the temperature further after the 2 heat exchangers, the pressure is reduced to 75 bar over a valve, exploiting the Joule-Thomson effect. The pressure after the valve is controlled by adjusting position of the blades in the subsequent expander. The power from this expansion function drives the compression of the top product. Trade of between the pressure drop and temperature drop over the valve, gives a possible internal minimum for the cost function of the system.

The liquid from the feed separator, stream 4, is cooled and expanded over a valve in to the cold separator. Vapor from the cold separator enters the column at the top stage and flows out with the distillate. The liquid from the cold separator is slit in two, stream 8 and stream 2. Stream 8 is used to to cool the feed to the cold separator and stream 8 is feed to the column at tray 23. The split ratio effect the behavior of the column. When the flow in stream 8 is increased more heat is transfered in the heat exchanger before the cold separator, decreasing the temperature of stream 5. The effect strengthen itself, as when the cold separator becomes colder, even more heat is transfered from stream 4 further reducing the temperature of the cold separator.

The bottom temperature in the column is controlled by manipulating the the re-boiler duty. The pressure in the column is not controlled.

The column has two side boilers. On is sited at stage 18, and is used to precool the gas entering the section. In some occasions this unit may cool the tray instead of heating. The other boiler is sited at stage 6 and the energy added is controlled.

2.1 Compression of sales gas

The distillate from the column is is called sales gas. This gas is in 3 parallels over the the sales gas compressors and the booster compressors. The gas is cooled between the two compression steps to increase the efficiency of the booster compressors. A simplified flow diagram for the compression section is presented in figure 2.2.

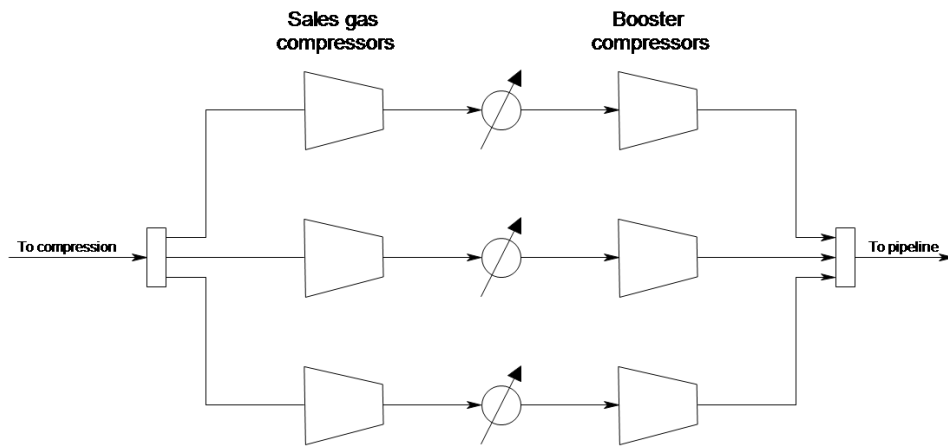


Figure 2.2: Flow diagram for the compression section

3 Creating a model in Unisim

Unisim is a simulator for chemical process plants developed by Honeywell. A steady state model of the methane extraction unit was developed in Unisim with the basis in the existing d-spice model and plant data. This was done to get a faster and hopefully more precise description of the system. UniSim also has the advantage that it can easily be connected and run by Matlab or another programming software through an actxserver. A flowsheet of the developed model is shown in appendix A. The specifications of the different units implemented in the model is given in table 3.1. Åsgard feed at a high rate is used as a basis for the parameters that was taken directly from the existing model in D-spice. The composition in the Åsgard feed is given in table 6.1. A detailed description of how the different parameters was found is given in appendix B. Peng Robinson was chosen as the equations of state, as it has been shown to describe hydrocarbon systems well [2].

Table 3.1: Specifications

Unit	Specifications	value
Heat exchangers		
21HA201	UA	$3.7 \text{ e}5 \text{ KJ/C h}$
21HA204	Temperature out	
Combined 21HA208/7/6	UA	$9.0 \text{ e}5 \text{ KJ/C h}$
Valves		
21HV2006A	Pressure out	
21LV2004	Pressure out	
21LV2001	Fixed pressure drop	1 bar
21LV2001	Controlled pressure drop	1 bar
Compressors and expanders		
Expander 21KA201	Polytropic Efficiency	0.75
	Pressure out	
Compressor 21KA202k	Polytropic efficiency	0.752
	Work from expander 21KA201	
All sales gas compressors	Polytropic Efficiency	0.74
	Pressure out	130 bar
All booster compressors	Polytropic Efficiency	0.77
	Pressure out	
Other		
Column 21VE103	Tray efficiency	0.8

3.1 Comments on the model derived

The real heat exchanger 21HA204 has a fixed UA and uses a bypass stream to adjust the heat transferred in the heat exchanger. The bypass is manipulated to keep Temperature out of the exchanger at its set point. In Unisim the temperature out is specified rather than UA . This is done as a bypass flow would require an adjust block that iterates in the flows until the temperature reaches the set-point. This greatly increases the time for the model to converge, and heightens the chance of convergence problems. To avoid that the modeled heat exchanger can transfer more heat than the real heat exchanger the parameters UA found from the d-spice heat exchanger is used as a constraint.

The compressor efficiency is taken directly from UniSim when the compressors are running

with Åsgard feed at highrate. D-spice uses the compressor curves from the real compressors to get a more precise behavior. Tries on implementing the same compressor curves in Unisim failed.

The in a real staged distillation column the liquid and vapor never reaches equilibrium. The tray efficiency in the UniSim model is a measure of how close to equilibrium each tray are. UniSim uses the Murphree stage efficiency presented in equation 3.1 [3]

$$E_n = \frac{V_n y_n - (V_{n+1} y_{n+1})}{V_n K_n X_n - V_{n+1} y_{n+1}} \quad (3.1)$$

Where

E : Efficiency

V_n : Total vapour molar flow leaving stage n

y : vapour mole fraction

$K_n X_n$: composition of vapor in equilibrium with the tray liquid

x : liquid mole fraction

n : tray number (measured top down)

The Murphree stage efficiency is the vapor composition leaving the tray over the vapor composition at equilibrium. It was attempted to tune the temperature profile to to plant data. Figure ?? shows the temperature profile of the demathanizer in train 200 01.05.2012 00:00:00, together with temperature data.

As the profile is very sensitive to small changes in the bottom temperature the comparison is done by setting the temperature by setting the temperature at tray 18 to plant data. Tray 18 is chosen as the temperature profile is very steep at this point. Thus minimizing measurement errors from the plant. Tray 18 also have the advantage that the top side boiler is on this tray. Adjusting the temperature on this tray then make sure that the energy inserted in this tray is closer to the real value.

The profiles from UniSim has from all the cases approximately the same shape as the plant data. However the temperature on all trays lower in UniSim than the real column. Figure 3.1 show that this is due to the much steeper temperature profile in the bottom of the unisim column than the real column. The large temperature drop indicate that the unisim has a to large tray efficiency. There are however close to no difference in to profile in the bottom of the column when the

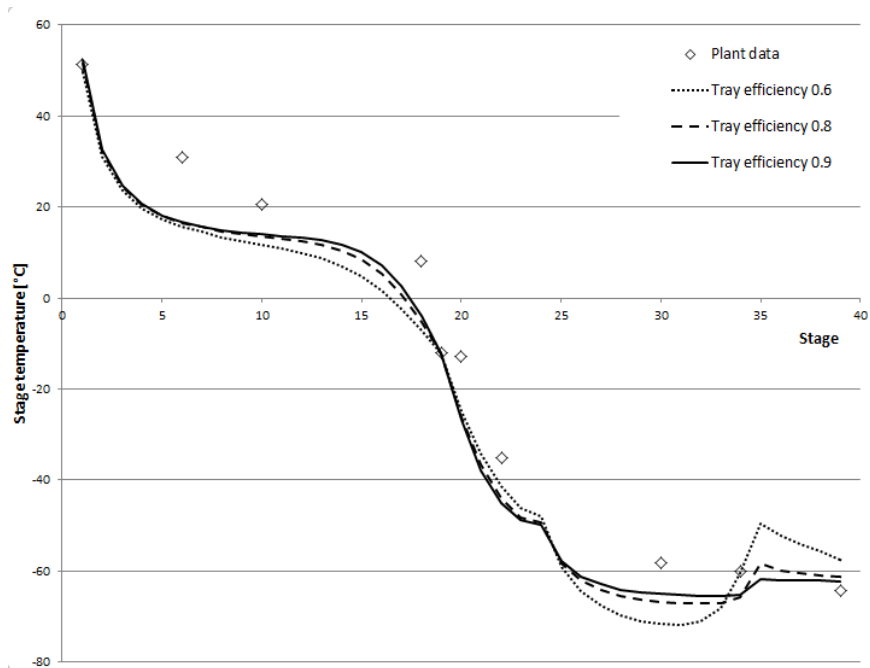


Figure 3.1: Temperature profile of the train 200 demethanizer together profiles from UniSim at different efficiencies. The trays of the column is counted from bottom to top

efficiency is changed.

4 Model verification

To verify that the model coincide with the real plant and the existing model in UniSim, a case study was conducted. The input and all the set-points in the d-spice and the UniSim model was set to match plant data for the T200 demetanizer at 01.05.2012 00:00:00. This is the same case as was used to study the effect on the tray efficiency, but from the case used when calculating parameters from D-spice. The boundary and set points used is presented in table 4.1 and table 4.2. Flow, pressure and temperature from calculated from UniSim is presented together with corresponding values from plant data and D-spice in table 4.3.

Table 4.1: Boundary conditions

Flow	3.90E+05	<i>kg/h</i>
Temp	3.2	<i>°C</i>
Pressure	115.5	<i>bar</i>
N	0.00673	<i>mol frac.</i>
Co2	0.02690	
C1	0.80465	
C2	0.09035	
C3	0.04693	
iC4	0.01165	
nC4	0.00656	
iC5	0.000000239	
nC5	0.000000237	
C6	0.000000229	
C6+	0.00000029	

Table 4.2: Set-points for validation case

TC Feed separator	-17.7	<i>°C</i>
PC feed separator	75 n bar	
PDC	2.4	<i>bar</i>
RC to column	0.59	
XC side boiler	2.6e5	<i>W</i>
TC column	51.4	<i>°C</i>
Pressure after expander	36.6	<i>bar</i>

Table 4.3: Comparison of the UniSim and Dspice to plant data

Feed to sec	Unisim	Dspice	Plant data
Flow	3.90E+05	3.90E+05	3.90E+05
Temp	3.2	3.2	3.2
Pressure	115.5	115.5	
1			
Flow	3.90E+05	3.90E+05	3.90E+05
Temp	-0.5	2.2	-5
Pressure	115.5	112.5	
1b			
Flow	3.90E+05	3.90E+05	3.90E+05
Temp	-17.5	-17.5	-17.5
Pressure	115.5		
3			
Flow	3.90E+05	3.90E+05	
Temp	-32.6	-31.9	
Pressure	75	75	75
13			
Flow	2.60E+05	2.70E+05	2.99E+05
Temp	-32.6	-31.9	
Pressure	75	75	75
4			
Flow	1.30E+05	1.23E+05	
Temp	-32	-32.2	
Pressure	75	74.9	
5			
Flow	1.30E+05	1.23E+05	
Temp	-51	-54	-69
Pressure	74.9	74.7	
6			
Flow	1.30E+05	1.20E+05	
Temp	-61.9	-64.6	
Pressure	37.4	37.2	
9			
Flow	4.68E+04	4.00E+05	6.50E+04
Temp	-61.9	-64	-73
Pressure	37.4	10 36.8	
2			
Flow	4.80E+04	3.70E+05	4.50E+04
Temp	-61.9	-64	
Pressure	37.4	37	

10			
Flow	7.00E+04		
Temp	-38	-40.9	-36
Pressure	35.6	35.1	
14			
Flow			
Temp	-63.6	-64.1	
Pressure	36.6	35.7	36.6
D			
Flow	2.70E+05	3.23E+05	
Temp	-61.2	-63.4	-64
Pressure	34.6	35.7	35.5
Methane	0.924	0.922	0.918
Ethane	0.04	0.045	0.044
Propane	0.006	0.0055	0.006
B			
Flow	1.20E+05	1.00E+05	
Temp	51.9	51	
Pressure	34.9		
Methane	0		
Ethane	0.388		
Propane	0.291		
CO2	0.0655		

The comparison conducted showed a relatively good match between the models and plant data. However there are for both models mismatches a few places. There are many possible causes for these errors. In general it is either caused by measurement errors from the plant, wrong parameters implemented in the models or that the model is not complex enough to describe the process. Below key matches and mismatches is discussed.

After the feed is cooled with a side stream from the column it becomes stream 1. Plant data show a temperature of at the $-5\text{ }^{\circ}\text{C}$, UniSim $-0.5\text{ }^{\circ}\text{C}$ and D-spice $2\text{ }^{\circ}\text{C}$. The UniSim model uses a only simple model with only the heat transfer coefficient UA as a adjustable variable. UA is expected to be function of the flowrate and temperature. As all the model parameters was found for a case with different boundary and initial conditions there there is expected to be some errors in all the heat exchangers. The D-spice model that uses a much more rigorous model has however a even

large error. This is due to the bad match between the temperature profile of the real column and the d-spice column, that causes the temperature of the side stream not to match with the plant data.

After heat exchanger 21HA204 the flow becomes stream 1b and the temperature heat transferred in the heat exchanger is adjusted to match plant data. The stream is then expanded over a valve in to a flash tank. Temperature and flows out of the flashtank have for both models a vary good match with plant data (Stream 13 gas and stream 4 liquid from flash). This indicate that the thermodynamic models that the to models uses works well.

The two models is quite similar in the system around the cold separator (stream 5 and 6 and 9), but have small differences to the plant measurement. The plant data shows a lower temperature for stream 5 and 9 for the 2 models. A the cold separator the Unisim and plant data match well. The D-spice how however much more as liquid face then the unisim and dspice model. As stream 5 is colder for both the D-spice and UniSim model for plant data there should theoretically be less liquid product then the the plant data. As both models behaves opposite of what the temperature measurement indicate there might indicate that some some of the plant measurement is not correct.

The Unisim model have a relatively good match on the flows to the column that is measured, stream 2 and 10 and 14. The D-spice model has a to lower flow in stream 2 then the plant data. The D-spice model and plant measurement shows a distillate temperature of about $-64\text{ }^{\circ}\text{C}$ and good compliance at the composition. The UniSim model have a distillate temperature of -61.2 , several degrees higher then plant data and D-spice. The gas flow to the column was in UniSim -64 so the differences has to be caused by the gas flow up trough the column. As the temperature is higher the plant data indicated that the tray efficiency was not good enough. When however the tray efficiency was turn up up to 100 % the temperature only decreased to -62 . The reason for the difference between the unisim and d-spice model is not known. It might be caused be errors in the thermodynamic model used by UniSim, small errors in the flow to the column that affect the temperature profile or wrong tray efficiency.

5 The real optimization problem

The objective of the study is to find the set-points on the current control structure, that gives the highest possible profit. Mathematically this is done by minimizing the cost function with respect to the constraints. The profit is maximized when the cost function is minimized. Only steady state effects have been considered and the prices in the cost function, p , is assumed to be constant.

5.1 The cost function

A full cost function for the demetaniser section in Train 100/200 is proposed in equation 5.1.

$$C = p_F F + p_{w_g} W_g + p_{w_{el}} W_{el} + p_V V + p_S S - p_B B + p_D D \quad (5.1)$$

Where p is the price of the utility or product used, and the capital letter is the amount used.

F : Feed to the section

W_g : Total compression work for the sales gas compressors

W_{el} : Total compression work for the booster gas compressors

V : Re boiler flow

S : Side boiler

D : Distillate

The optimization later is done under the assumption of fixed feed. The feed part of the cost function is then constant and will not influence the set of optimal states. Thus the feed part of the cost function can be taken out of the equation. The prices, p , in the cost function is not accessible and has to be estimated. The estimation of prices is done in section 5.2.

5.2 Derivation of the cost function parameters

The sales gas and liquid product price:

The marked price for sales gas is assumed to be approximately 0.390 NOK/kg and the bottom product price is set to 1.0 NOK/kg. The liquid product price p_B is the price of selling the liquid products after the cost of the further processing is withdrawn [5].

The price for compression work $p_{w_{el}}$ and p_{w_g}

The sales gas compressor is driven by burning sales gas. It is chosen to use the power input to the compressor calculated by Unisim as a basis for the cost calculations of the compressors. Assuming that all the energy from burning sales gas can be utilized for compression. The price of the sales gas compressors per power input can then be calculated by equation 5.2.

$$p_{w_g} = \frac{p_c}{\Delta_c H} \quad (5.2)$$

The price of sale gas, p_c , is the estimated to 0.390 *NOK/kg* and $\Delta_c H$ is the combustion enthalpy of sales gas. The sales gas consist primarily of methane which has the a combustion enthalpy of 890 *kJ/kg*. The price of using the sales gas compressors then becomes 4.4 e-4 *NOK/kJ*. This price is under the assumption of 100% efficiency in the motor driving the compressor. The real price is much higher.

The booster compressors is powered by electricity. The spot price for electricity 7. December 2012 on the west coast of Norway was 1.2 e-4 *kr/kJ* [?]. It is chosen to be conservative and use the sales gas price p_{w_g} for all the compression work as that price is highest.

The reboiler energy price p_B

The reboiler is powered by burning sales gas. The price of the reboiler p_V can roughly be estimated by rearranging the energy balance and multiplying by the gas price, equation 5.3. Energy loss in the transfer of energy is not taken in to account.

$$p_V = p_c \frac{\Delta_{vap} H_V}{\Delta_c H} \quad (5.3)$$

$\Delta_{vap} H_V$ is the heat of vaporisation for the bottom product. The bottom product is a mixture mainly consisting and ethane, CO_2 and propane. For simplicity the heat of vaporisation of ethane has been used. $\Delta_{vap} H_V$ for ethane has the value 50 *kJ/kg* [4]. p_c is the price of sales gas with the value of 0.390 *NOK/kg*, and $\Delta_c H$ the combustion enthalpy of methane with the value 890 *kJ/kg*. The price of the reboiler with respect to the boilup V then becomes 0.022 *NOK/kg*.

5.3 Cost function with prices

The cost function with the calculated prices is presented in equation 5.4. Notice that the cost of the feed is taken out as the optimization is done for a given feed. The sales gas and the booster

compressor is multiplied in to one therm, where p_w is the total compression work.

$$C = 0.00044W + 0.022V - 1.0B + 0.39D \quad (5.4)$$

5.4 Constraints

To find the optimal operation point the cost function has to be minimized with respect to the plant constraint. Material, process and product limitations is considered. The constraint for the demetanizer section is presented in table 5.1.

Table 5.1: Limitations

Tag	Description	Limit
Material constraints		
21PC1006	Tower pressure	<36 bar
21PC1002B	Expansion pressure	<78 bar
21TI1022	Temperature stage 19	>-30°C
Other constraints		
21PDC1001	Pressure diff. coldsep. Tower	1%<u<100%
	Temperature before compressor	<-35°C
22XC0004	Suction pressure sales gas	<45 bar
	Rpm sales gas compressor	<100/105
	Rpm booster compressor	<100/105
	Exit pressure booster compressor	<191.7 bar
	Burne temperature sales gas compressors	< 670 °C
Product specifications		
	Methane in bottom	<1 mol%

5.5 Degrees of freedom

The cost function are to be minimized by adjusting on the degrees of freedom. The current controllers is used as the degrees of freedom, is listed in table5.2.

Table 5.2: Controlled variables in the demethanizer

Controlled variable	Manipulated variable
Entering temperature expansion sep.	Amount bypass heat exchanger of distillate
Pressure expansion sep.	Blades in expander?, affects energy to compressor
Ratio split liquid from cold separator	Valve
Pressure diff. cold sep- tower	Valve
Energy input side boiler	Flow hot side heat exchanger
Tower bottom temperature	Level liquid hot side
Suction pressure to section7	Not controlled

6 Study of the model

The model derive in UniSim is studied with Åsgard rich gas feed. The composition of the feeds is presented in table 6.1.

Table 6.1: Composition of the Statpipe and Åsgard rich gas

Component	Åsgard rich gas [mol%]
CO2	2.60
C1	79.77
C2	9.56
C3	4.75
IC4	0.70
NC4	1.18
IC5	0.28
NC5	0.26
C6	0.15
C7	0.12
C8	0.05

The following specifications in the feed was used for all the cases studied:

Flow 4.0e5 kg/h

Pressure 115.5 bar

Temperature 5 °C

The model was studied by systematically changing the degrees of freedom corresponding to the controllers of the real plant. When one degree of freedom was changed, the other was fixed at a chosen normal value. The chosen normal values is presented in table 6.2 together with the range it was changed over. Notice that pressure after the expander is specified instead of the suction pressure section 7. This will not affect the optimal operation point, and is done because UniSim need to have specified the column top and bottom pressure. The effect of changing the pressure after the expander is not studied. This is not done as the bottom column pressure is not made a fuction of the top pressure.

Table 6.2: Degrees of freedom for the chosen normal operation conditions

Degree of freedom	Normal value	Range	Unit
TC Feed separator	-14.5	[-24 -14]	°C
PC feed separator	74.65	[60 78]	bar
PDC	2.6	[0.5 8]	bar
RC to column	0.50	[0.2 0.8]	
XC side boiler	2.5e5	[0 4e5]	kJ/h
TC column	54	[45 60]	°C
Pressure after expander	43.3		bar

6.1 Effect of changing the column bottom temperature

The column bottom temperature was changed, keeping all other degree of freedom constant. How separate elements of the cost function, CO₂ in the desillate and methane in the bottom product is changing is plotted in figure 6.1. The constraint on keeping the the temperature on tray 19 over 30 °C is breached when the bottom temperature go bellow 48 °C.

When the column bottom temperature increases the the amount of the bottom product (B) decreases and amount of top product (D) increases. The income from the top and bottom product is proportional to the amount. As the amount of top product increases the cost of the compression go up. The plot shows that the cost function is changing the most right after the constraint and is quite flat in the infeasible region. This shows that it is not so much to save by moving the in to the infeasible region.

In a distillation column purity constraint on expensive products is almost always active [6]. This is to avoid product give away and save energy in the re-boiler. In the demetanizer the bottom product is much more valuable than the top product, 0.39 *NOK/kg* for top and 1.0 *NOK/kg* for bottom product. The bottom product is specified to have concentration of methane less then 1 %. The plot of the methane concentration in figure 6.2 shows that is not possible to get a concentration of methane in the bottom without breacing the temperature constraint on tray 19. The pairs of methane and temperature conditions under normal operation conditions is presented in table 6.3.

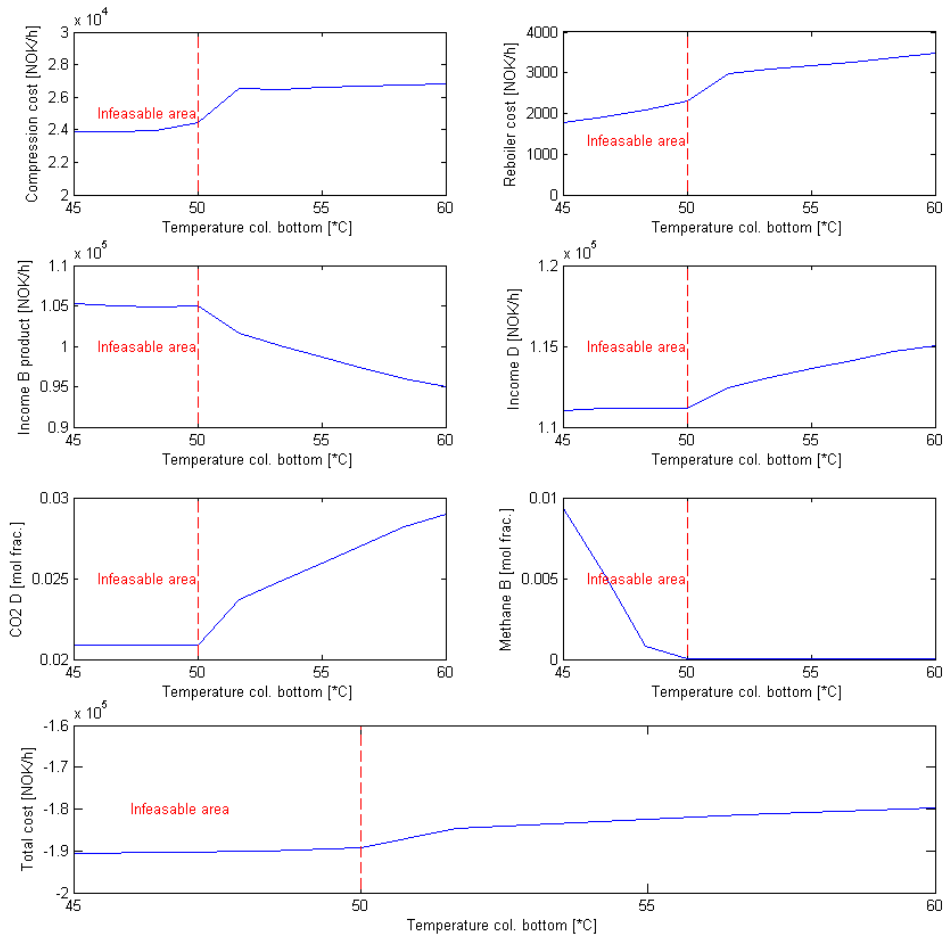


Figure 6.1: Effect on the cost function and column product concentration, by changing the column bottom temperature

Table 6.3: Active constraints in column

Case	Temperature bottom[°C]	Temperaure tray 19	Bottom composition methane [mol%]
1	45.0	-42.7	1.0
2	48.0	-30	2.3e-5

The minimum cost is at the temperature constraint. In the rest of the rest of the study the

temperature on tray 19 is fixed to 30 °C instead of the bottom temperature. This is to get the most correct information of where the global optimum for the cost function are.

6.2 Effect of changing the temperature before the feed separator

The temperature before the feed separator is changed in the range -24 °C to -14 °C. The effect of the cost function, CO₂ in to and Methane in top is presented in figure 6.2

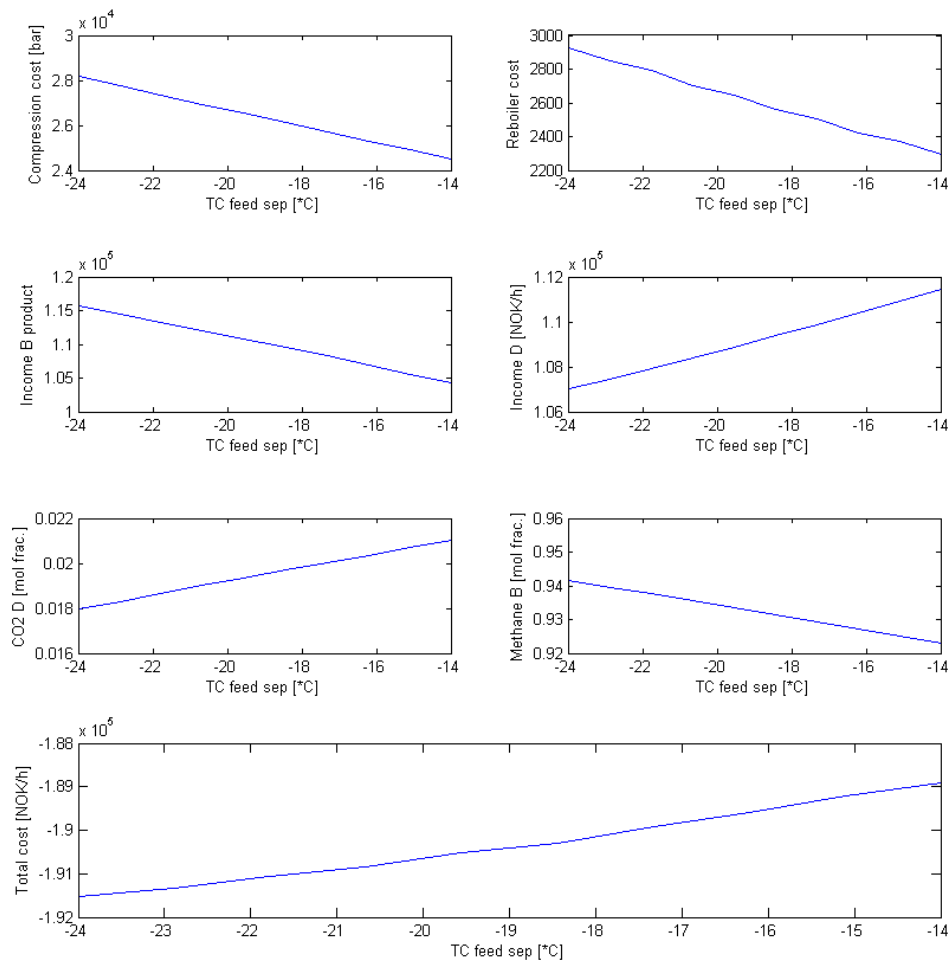


Figure 6.2: Effect on the cost function, top methane composition and top CO₂ composition, when changing the temperature before the feed separator

When the temperature in before the feed separator decreases the amount of liquid from the feed separator increases. This leaves less gas to drive the turbo expander (21KA201), and less work is available on the compression side. However when the temperature in the temperature before the feed separator is decreased not as much heat is transferred from the distillate keeping the temperature on the compression side low. When the temperature is low less work is needed for the pressure increase.

The simulation shows that the CO₂ in top is slightly increasing when the temperature before the feed sep increases. The CO₂ concentration should be kept as low as possible. As the total cost is also at its lowest value when the temperature is low, it is probable optimal to keep the the temperature as low as possible before the feed separator.

6.3 Effect of changing the pressure before expansion

The pressure before the feed separator, equal to the pressure in the feed separator, was changed in the range 60 to 78 bar. The effect on the cost function is plotted and presented in figure 6.3. The pressure has to be kept below 78 bar due to a constraint.

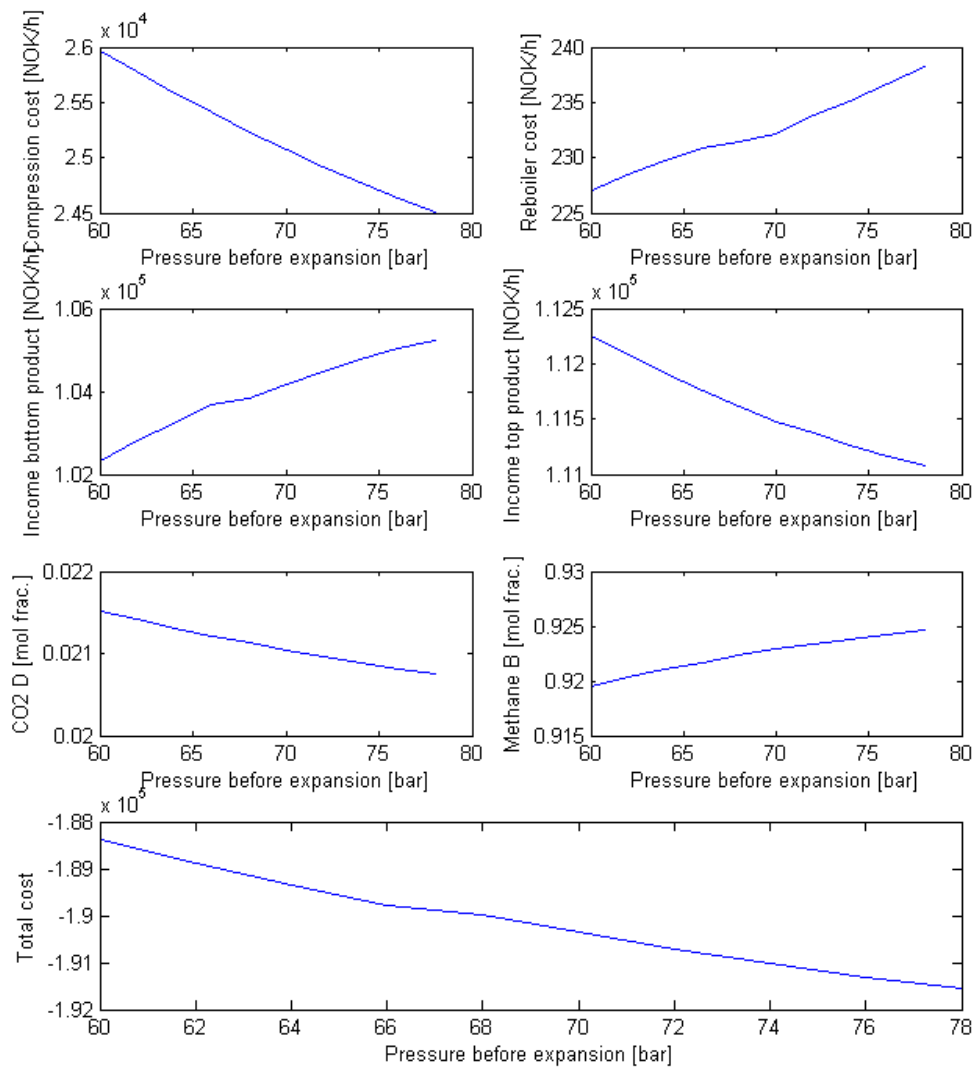


Figure 6.3: Effect on the cost function, top methane composition and top CO₂ composition, when changing the pressure before expansion

When the pressure in the feed sep decreases the amount of liquid increases. Figure 6.3 shows that the cost function decreased from $-1.88.5e6$ *NOK/h* at 60 *bar* to $-19.5e5$ *NOK/h* at the constraint of 78 *bar*. Thus it is optimal to be at constraint.

6.4 Effect of changing the pressure diff. cold sep. to column

The pressure drop between the cold separator and the tower (stream 36 and 12) was changed in the range [0.5 8] bar. The effect is presented in figure 6.4

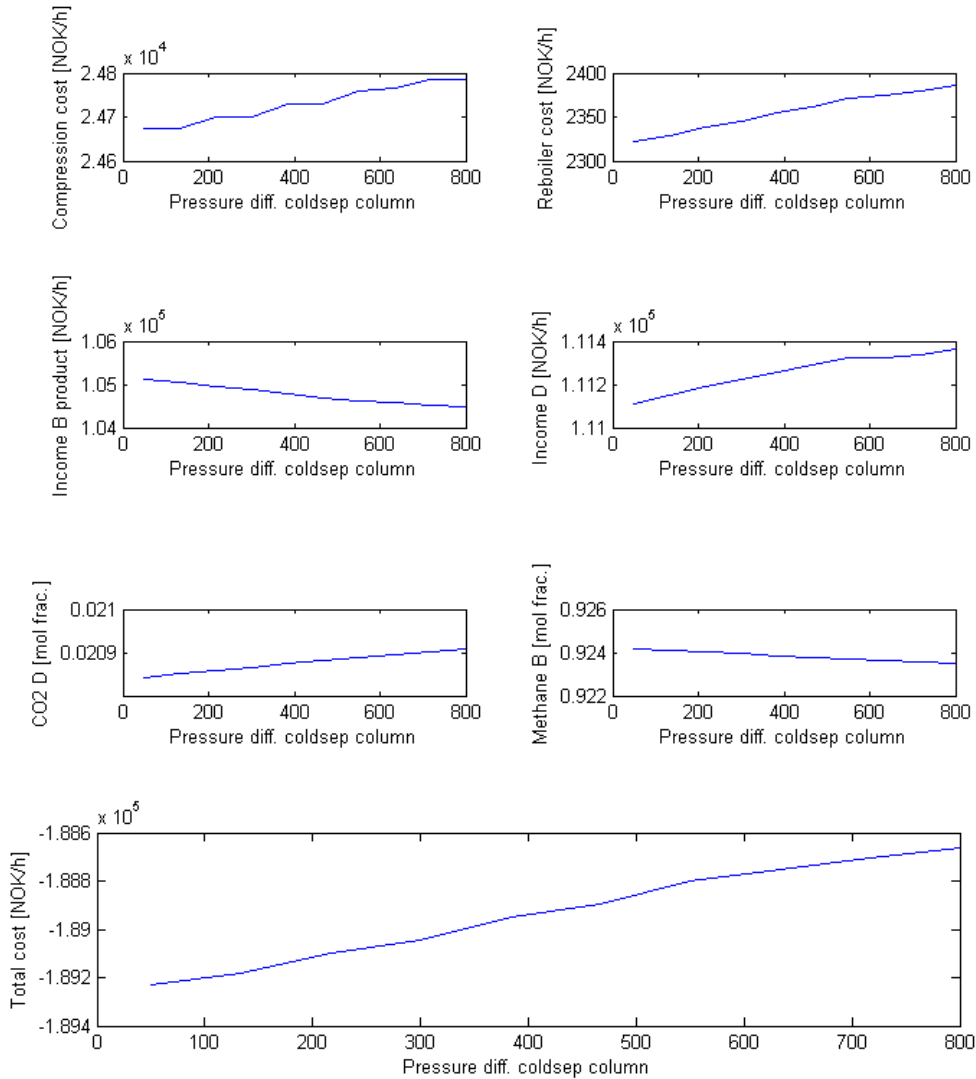


Figure 6.4: Effect on the cost function, top methane composition and top CO2 composition, when changing the pressure drop between the cold separator and the column

There is close to no change in the cost function when the pressure drop is changed. The cost is decreasing marginal with decreased pressure drop. On the real plant there are a constraint on the on the valve opening. The valve has have a opening over 1% and under 99% opening, see table 5.1. This pressure drop is controlled by adjusting the valve opening. As the cost is lowest for the lowest pressure drop the valve should open as much as possible. However the pressure in the real column is not controlled. This effect is simulated by assuming a pressure difference of 0.2 *bar* between stream 14 and 12. The pressure in the cold separator is not effected by the pressure drop between the cold sep and the column as the real plant would. This differences between the real plant and the model make it difficult to draw any conclusion on the ideal set point for the pressure drop controller.

6.5 Effect of changing the power in the side boiler

The power input in the side boiler was changed in the range 0 to $4e5 \text{ kJ/h}$ The effect on the cost function is presented in figure 6.5

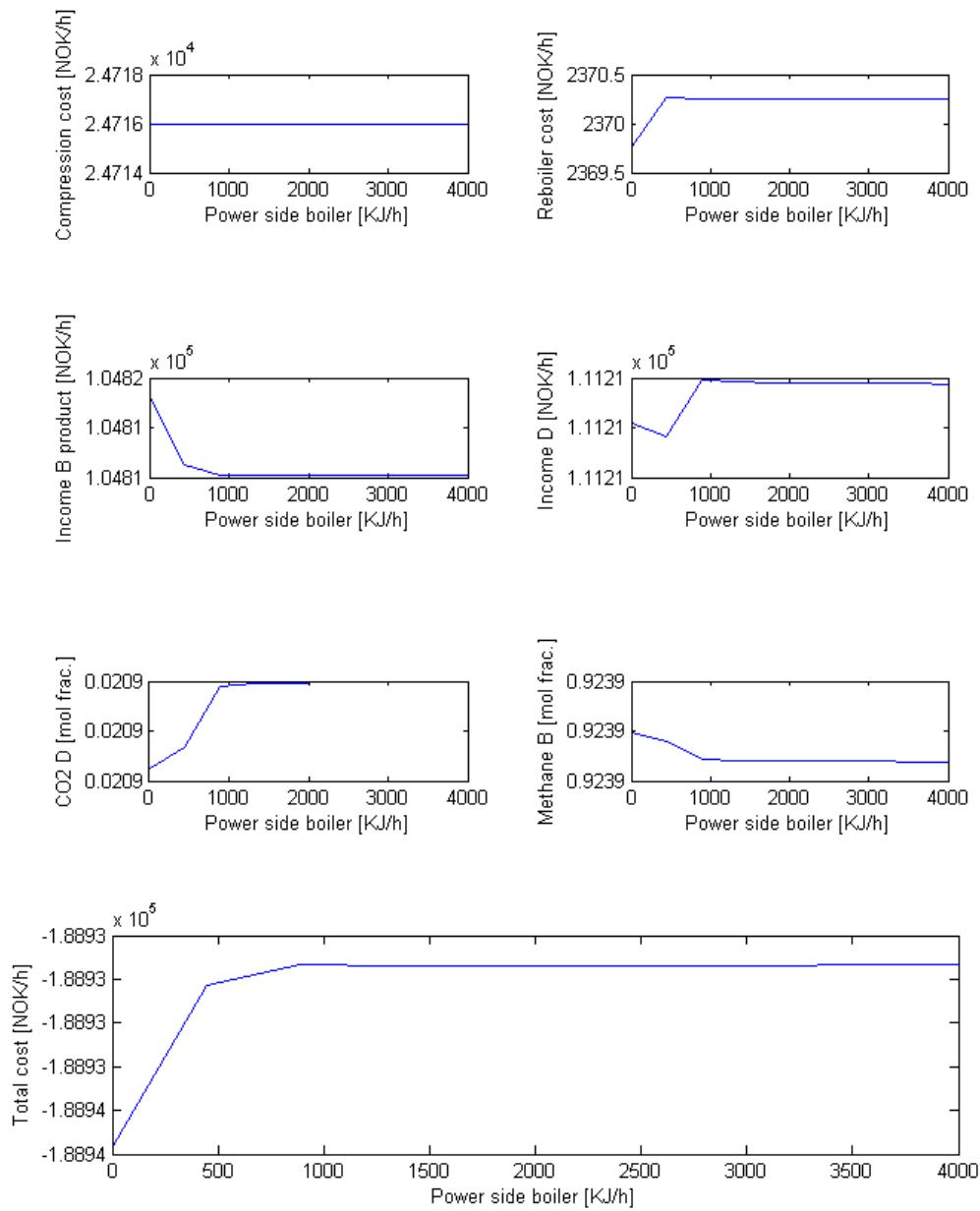


Figure 6.5: Effect on the cost function, top methane composition and top CO₂ composition, when changing power to the side boiler

When the energy input in the side boiler increases the re-boiler cost decreases marginally, as shown in the top right plot in figure 6.5. Theoretically as the energy input in the side boiler increasing a separation done in the steps below the side boiler is decreased. Thus the total energy to the column has to increase to have the same total separation. This might be why there is nearly no effect of increasing the energy in the side boiler even as the energy to the side boiler is assumed to be free.

6.6 Effect of changing the split of liquid form the cold separator

The liquid from the cold separator is split in two. The fraction of the flow that is feed directly in to the column (stream 2) is changed over the range 0.2 to 0.8. The effect on the cost function and presented in figure 6.6

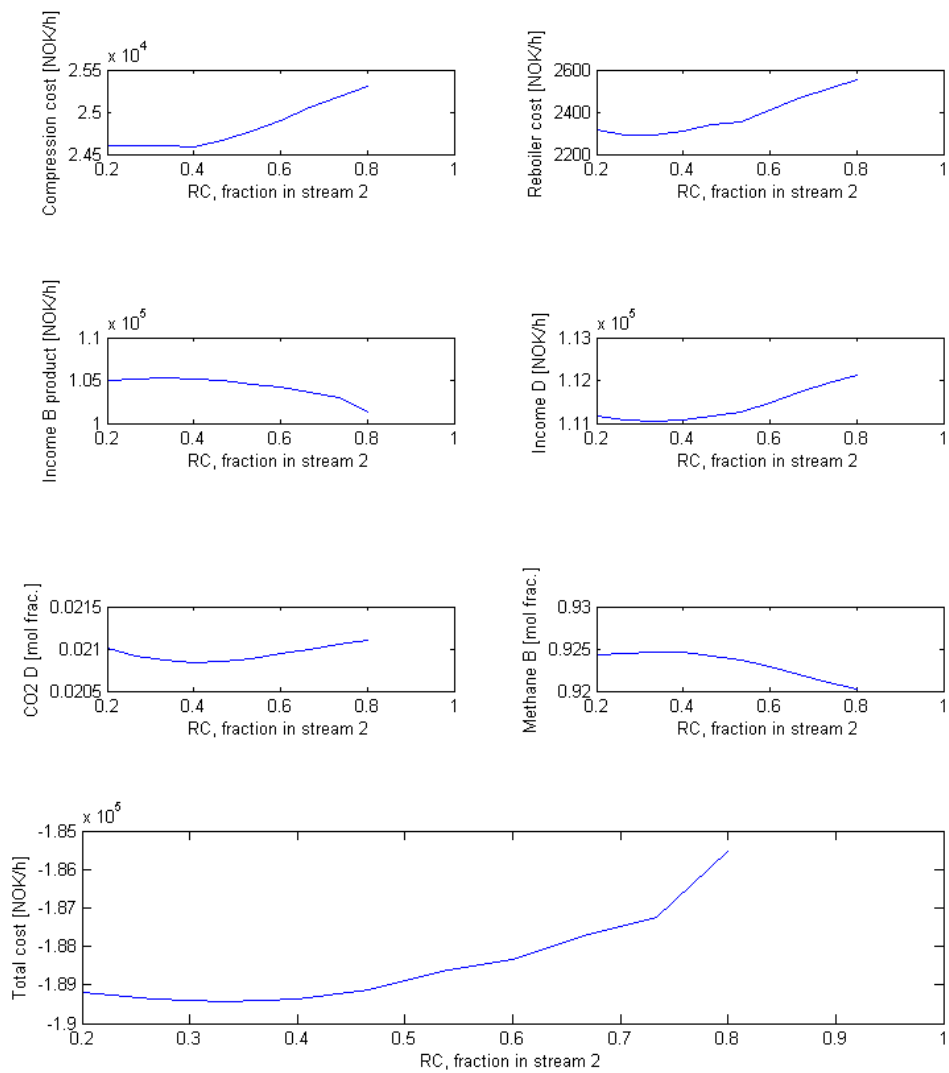


Figure 6.6: Effect on the cost function, top methane composition and top CO₂ composition, split of the liquid from the cold separator

The simulation shows an internal minimum of the cost function when a about 33 % of the liquid is feed at the top tray. However the cost function is relatively flat when chaining the slit ratio, only amount 4500 is saved by operating the plant at 33 % compared to 80 %.

7 Attempt on automated optimization

It was attempted to use a minimization solver in Matlab to find the global minimum of the cost function. A none derivative based numerical solver was used to avoid problems when numerical derivatives is to be calculated by making small changes in UniSim. The Matlab files used is presented in appendix D. The solver crashed after about 5 iterations as UniSim was unable to converge. UniSim did not converge because the flow to some of the heat exchanger had become to small. It was attempted to implement constraints on the flows, restrict them from becoming to small. However the attempt failed as the streams still become to small. It is possible that the solver is implementing a large step over the constraint before it would contradict to the constraint border. Smaller step length and larger values for the constraint on the streams might solve the problem. This would however greatly increase the runtime of the program.

8 Discussion

8.1 The UniSim model

The model derived showed a reasonable match with the real plant and the d-spice model. The model was however only validated at one case. This decreases the trust in the models accuracy, and it is not known how well the model describes the case studied in the optimization. Due to the behavior of UniSim the model had to be made by specifying the pressure drop between the stream from the expander and the distillate, and the bottom pressure needed to be fixed. In the plant the pressure is floating. This inequalities to the real plant will give a difference in the optimal operating point for the model and for the plant. There was also many of the constraint that in the real plant that was not simulated by UniSim. Further study has to be done to to investigate if it is possible to the the the optimal set-points found in this study.

8.2 The study of the model

For the case studied, the column temperature and the pressure before the expander showed to have its minimum value for the cost function, at the constraint. It is then ideal to control the process so this constant are fixed at the constraint. An internal minimum for the cost function was found when changing the split of liquid from the cold separator (RC). The minimum was found at RC equal to 0.33. Disturbances will might change this optimal value. This might be changes in the feed flow rate, composition, the set-point for the other controllers, or prices in the cost function. In the calculation of the prices for compression and re-boiler usage it was assumed that 100% of the combustion energy could be utilized. The real cost of compression and re-boiler is then higher. This it would probable move the optimal value of RC slightly down, as figure 6.6 shows that the re-boiler and compression cost is nearly constant when adjusting RC down from the optimum, but increasing when adjusting RC up. The temperature of the the flow from the feed separator to the cold separator would also probable have great influence on the optimal RC set-point.

9 Conclusion

The simulated model of the demethaniser in train T100/T200 showed reasonable correlation with plant data and the existing model in D-spice for one case. As the model was only validated for one case, little trust can be given to the model when exposed to large changes in the operating and boundary conditions. The model was optimized for with a cost function found by market data, as the real prices are considered restricted information. Two active constraint was found. The pressure before expansion has its optimal value at the boundary of 78 *bar* and the column bottom temperature has its optimal when the temperature at tray 19 is kept at -30 °C. The temperature before the feed separator is found to be kept as low as possible. An internal minimum was found for the split of liquid from the cold separator. It was found that the optimal was to send 33% of the flow directly to the top of the column. The minimum for the split will is dependent on how good the model and the cost function are.

References

- [1] "<http://www.gassco.no/wps/wcm/connect/gassco-en/gassco/home/var-virksomhet/prosessanlegg/karsto/karsto>, Sited: 10. Desember 2012.
- [2] Dont gamble with physical properties for simulations. [http://www.eq.uc.pt/~nuno/eps/old/2010-11/aula09/Carlson%20\(1996\).pdf](http://www.eq.uc.pt/~nuno/eps/old/2010-11/aula09/Carlson%20(1996).pdf), Sited: 21. April 2012.
- [3] UniSim deign R400. program help page, 2012.
- [4] Findlay. SI Chemical data. Wiley, 5th edition edition, 2002.
- [5] Marius Govatsmark. personal communication, 2012.
- [6] Sigurd skogestad. plantwide2-cv1-selection-soc.ppt,<http://www.nt.ntnu.no/users/skoge/vgprosessregulering/lectures/>, 2012.

Appendices

A Flowsheet of the UniSim model

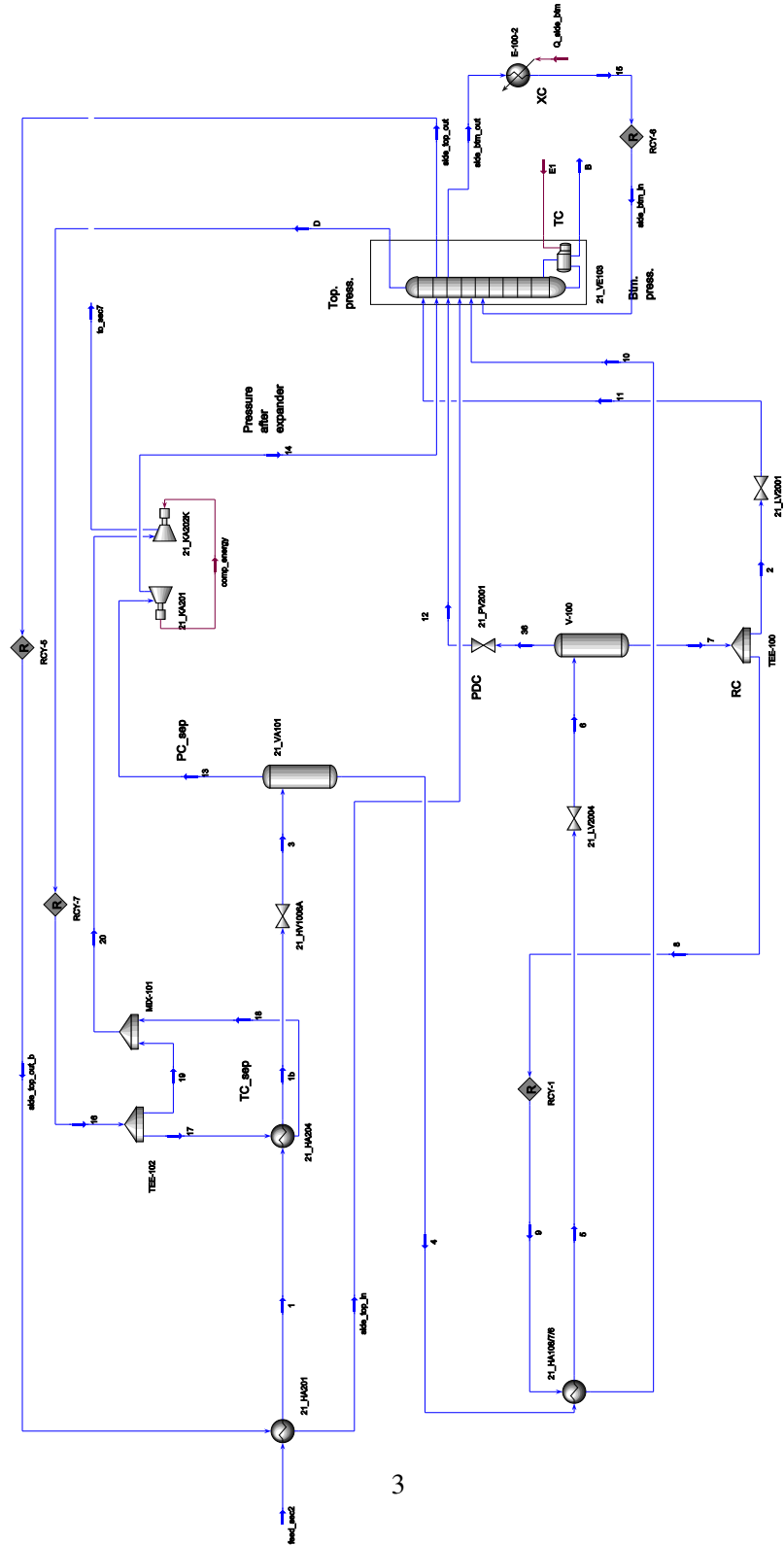


Figure A.1: Flowsheet of the UniSim model

B Derivation of the Unisim model parameters

A Unisim model of the the demethanizer section at Kårstø was developed with the basis in the existing dynamic simulator in D-spice and plant data. The derivation of the parameters in the model was developed with the basis in Åsgard high rate feed under normal operating conditions. The composition of the feed used is presented in table B.1

Table B.1: Entering feed compositions

Component	Mas fraction
H2O	0
N	0
CO ₂	2.6
C1	79.77
C2	9.56
C3	4.75
iC4	0.7
nC4	1.18
iC5	0.28
nC5	0.26
C6	0.15
C7	0.12
C8	0.05

The operation conditions in the case used to find the parameters is presented in table B.2

Table B.2: Entering feed compositions

Component	Mas fraction
Feed flow rate	400000 <i>kg/h</i>
Feed Temperature	5 °C
Feed pressure	115.5 <i>bar</i>
Entering temperature expansion sep.	-18 °C
Pressure expansion sep.	75 <i>bar</i>
Ratio split liquid from cold separator	0.67
Pressure diff. cold sep tower	2.4 <i>bar</i>
Top pressure methane tower	32.2 <i>bar</i>
Energy input side boiler	2.5 <i>MJ/h</i>
Tower bottom temperature	54 °C
Suction pressure to sec 7	41.5 <i>bar</i>

B.1 The heat exchangers

The heat transferred in the UniSim heat exchangers is calculated by equation equation B.1

$$Q = fUA\Delta T_{lm} \quad (\text{B.1})$$

Q is the heat flow rate, UA is the overall heat transfer coefficient and f is factor correcting for not ideal countercurrent flow. The logarithmic mean temperature ΔT_{lm} is shown in equation B.2

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\log \frac{\Delta T_1}{\Delta T_2}} \quad (\text{B.2})$$

Where ΔT_i is the temperature difference at the outlet and inlet of the heat exchanger. Data for calculating UA taken from is taken from UniSim and presented in table B.3.

Table B.3: Heat exchanger parameters

	21HA201	21HA204	21HA108-6
ΔT_1 [$^{\circ}\text{C}$]	7.8	9.2	9.7
ΔT_2 [$^{\circ}\text{C}$]	8.5	45.3	10
ΔT_m [$^{\circ}\text{C}$]	8.2	22.7	9.8
Q [kW]	816	10393	2465
UA [kW/K]	99.3	458	250
$\Delta P, \text{tube side}$ [bar]	0.9	0.1	0.1
$\Delta P, \text{shell side}$ [bar]	0.03	0.35	1.8

To avoid a too rigorous model that might have convergence problems at some operating conditions, the pressure drop is set to zero for most of the heat exchangers. The heat transfer coefficient UA is specified in the UniSim model for heat exchanger 21HA201 and heat exchanger 21HA108-6. For heat exchanger 21HA204 temperature out has been used as a specification as this is a controlled parameter at Kårstø. In the plant the temperature is controlled by bypassing parts of the distillate around the heat exchanger. When the temperature out of the heat exchanger is specified UniSim calculates the heat transfer coefficient UA needed. To avoid that the modeled heat exchanger can transfer more heat than the real plant, the heat transfer coefficient presented in table B.3 is used as a constraint.

C Comparison of the UniSim and Dspice to plant data

The model developed in unsim was compared to the existing model in dspice and plant data. Data from train 200 at 01.05.2012, 00:00:00 was used. The two models was fitted to plant data by setting the same boundary and controller set points, as the plant data. The set-point and boundary conditions used is presented in table C.1 and table C.2.

Table C.1: Boundary conditions

Flow	3.90E+05	<i>kg/h</i>
Temp	3.2	<i>°C</i>
Pressure	115.5	<i>bar</i>
N	0.00673	<i>mol frac.</i>
Co2	0.02690	
C1	0.80465	
C2	0.09035	
C3	0.04693	
iC4	0.01165	
nC4	0.00656	
iC5	0.000000239	
nC5	0.000000237	
C6	0.000000229	
C6+	0.00000029	

Table C.2: Set-points for validation case

TC Feed separator	-17.7	<i>°C</i>
PC feed separator	75 n	bar
PDC	2.4	bar
RC to column	0.59	
XC side boiler	2.6	MW
TC column	51.4	<i>°C</i>
Pressure after expander	36.6	bar

Flow pressure and temperature for all streams in the process is compared. The data is presented in table C.3. Plant data is added where there are available either from direct measurement or if

it follows an direct due to mass balance.

Table C.3: Comparison of the UniSim and Dspice to plant data

Feed to sec	Unisim	Dspice	Plant data
Flow	3.90E+05	3.90E+05	3.90E+05
Temp	3.2	3.2	3.2
Pressure	115.5	115.5	
1			
Flow	3.90E+05	3.90E+05	3.90E+05
Temp	-0.5	2.2	-5
Pressure	115.5	112.5	
1b			
Flow	3.90E+05	3.90E+05	3.90E+05
Temp	-17.5	-17.5	-17.5
Pressure	115.5		
3			
Flow	3.90E+05	3.90E+05	
Temp	-32.6	-31.9	
Pressure	75	75	75
13			
Flow	2.60E+05	2.70E+05	2.99E+05
Temp	-32.6	-31.9	
Pressure	75	75	75
4			
Flow	1.30E+05	1.23E+05	
Temp	-32	-32.2	
Pressure	75	74.9	
5			
Flow	1.30E+05	1.23E+05	
Temp	-51	-54	-69
Pressure	74.9	74.7	
6			
Flow	1.30E+05	1.20E+05	
Temp	-61.9	-64.6	
Pressure	37.4	37.2	
9			
Flow	4.68E+04	4.00E+05	6.50E+04
Temp	-61.9	-64	-73
Pressure	37.4	9 36.8	
2			
Flow	4.80E+04	3.70E+05	4.50E+04
Temp	-61.9	-64	
Pressure	37.4	37	

10			
Flow	7.00E+04		
Temp	-38	-40.9	-36
Pressure	35.6	35.1	
14			
Flow			
Temp	-63.6	-64.1	
Pressure	36.6	35.7	36.6
D			
Flow	2.70E+05	3.23E+05	
Temp	-61.2	-63.4	-64
Pressure	34.6	35.7	35.5
Methane	0.924	0.922	0.918
Ethane	0.04	0.045	0.044
Propane	0.006	0.0055	0.006
B			
Flow	1.20E+05	1.00E+05	
Temp	51.9	51	
Pressure	34.9		
Methane	0		
Ethane	0.388		
Propane	0.291		
CO2	0.0655		

D Matlab scripts

Some of the matlab script that is used in the simulation is found in the following sub chapters.

D.1 Optimaliser.m

Main Matlab script running the other scripts.

```
%% Optimaliser.m
% Summary:
% author:      Tor Anders Marvik
% organization: Department of Chemical Engineering, NTNU, Norway
% contact:     torandma@stud.ntnu.no
% requires:    matlab
% version:     1.0
% todo 1.0:    Debugging "There is allways a second bug"
% started     Oktober 2012
%%

clc
clear all

serv = actxserver('UniSimDesign.Application');
hyCase = serv.ActiveDocument;                                %unisim model

% %=====ATTEMPTS ON AUTOMIZED OPTIMIZATION=====
%run('C:\Program Files\MATLAB\R2012a\toolbox\optim\optim\opti_Install')
%needs to be ran every time matlab is reopend as the installation
%do not save. Why????

% % TC_feed  PC_feed    PDC    RC_to_col  XC    TC_col  Pressure afte expander
% lb=[-19,    7500,    240,    0.67,    2.5e5,  54,    3400];
% ub=[-14,    8000,    500,    1,        4e5,    60,    3430];
% x0=[-18,    7500,    240,    0.67,    2.5e5,  54,    3430];
%
% %constraints= [p_top, T_stg19, c1_btm min stream constraints]
% d=[-3.5000 10 1,-3e4,-1e4,-1e4]'; %c<=d
%
%
% prob=optimprob('fun',@(x) cost_function(x,hyCase), 'nlcon',@(x) constraints(x,hyCase),...
```



```

%          'nlrhs',d,'bounds',lb,ub,'x0',x0);
% opts1 = optiset('solver','nomad','display','iter');
% Opt1 = opti(prob,opts1);
%
% [x,fval,exitmerke,info] = solve(  Opt1,x0)
%=====

%=====SYSTEMATIC SEARCH IN UNISIM=====

init=struct('init',-1);
data_all=struct('feed_sec2',init,'s1',init,'s2',init,'s1b',init,'s3',init,'s4',init,'s5',init,
               's6',init,'s7',init,'s8',init,'s9',init,'s10',init,'s11',init,...
               's12',init,'s13',init,'s14',init,'s15',init,'s16',init,'s17',init,...
               's18',init,'s19',init,'to_sec7',init,'D',init,'B',init,'side_btm_out',init,...
               'side_btm_in',init,'side_top_out',init,'side_top_in',init,...
               'constraints',init,'cost_parameters',init);
x=[-17.7,    7500,    240,    0.59,    2.6e5,  51.4,    3660];
data=[zeros(1,5),zeros(size(x)),zeros(1,8),zeros(1,39),0]; %initilize lenght of data

%  TC_feed  PC_feed    PDC    RC_to_col  XC    TC_col  Pressure afte expander
% x=[-14.5,    7465,    260,    0.5,    2.5e5,  54,    3430];
% TC_feed_change=linspace(-24,-14,10);
% for i=1:length(TC_feed_change)
%     x(1,1)=TC_feed_change(i);
%     [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
%     data=[data; cost_parameters,x,c, Temp_profile, merke];
% end
%

% x=[-14.5,    7465,    260,    0.5,    2.5e5,  999,    3430];
% pc_feed=linspace(6000,7800,10); %expansion pressure max 78 bar
% for i=1:length(pc_feed)
%     x(1,2)=pc_feed(i);
%     [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
%     data=[data; cost_parameters,x,c, Temp_profile, merke];
%
% end

%
% x=[-14.5,    7465,    260,    0.5,    2.5e5,  54,    3430];

```

```

% PDC=linspace(50,800,10);
% for i=1:length(PDC)
%     x(1,3)=PDC(i);
%     [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
%     data=[data; cost_parameters,x,c, Temp_profile, merke];
% end
%
% x=[-14.5,    7465,    260,    0.5,    2.5e5,  54,    3430];
% RC_to_col=linspace(0.2,0.8,10);
% for i=1:length(RC_to_col)
%     x(1,4)=RC_to_col(i);
%     [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
%     data=[data; cost_parameters,x,c, Temp_profile, merke];
% end
%
% x=[-14.5,    7465,    260,    0.5,    2.5e5,  54,    3430];
% XC=linspace(0,4000,10);
% for i=1:length(XC)
%     x(1,5)=XC(i);
%     [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
%     data=[data; cost_parameters,x,c, Temp_profile, merke];
% end
%
%
% x=[-14.5,    7465,    260,    0.5,    2.5e5,  54,    3430];
TC_col=linspace(45,60,10);
for i=1:length(TC_col)
    x(1,6)=TC_col(i);
    [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
    data=[data; cost_parameters,x,c, Temp_profile, merke];
end
end
%
%To se the effect of chaning the pressure after the exapnder, comlumn
%bottom pressure has to be made a fuctinon of the pressure after the
%exapander. Not done
% x=[-14.5,    7465,    260,    0.5,    2.5e5,  54,    3430];
% p_exp=linspace(3000,4000,10);
% for i=1:length(p_exp)
%     x(1,7)=p_exp(i);
%     [cost_parameters,merke,c,Temp_profile,data_all]=cost_function(x,hyCase,data_all,i);
%     data=[data; cost_parameters,x,c, Temp_profile, merke];
% end

```

```

%=====PLOTTING=====
[TC_col,RC]=meshgrid(linspace(45,50,5),linspace(0.3,0.7,5));
cost=zeros(5:5);

switch i
case 1
    for i=1:5
        for j=1:5
            x(6)=TC_col(i,j);
            cost(i,j)=cost_function(x,hyCase)
        end
        x(4)=RC(i,j);
    end

    figure(1)
    surf(TC_col,RC,cost)
    xlabel('Bottom temp column')
    ylabel('Split liquid cold separator')
    zlabel('Cost')
    contour(TC_col,RC,cost)

case 2
    x=[-14.5, 7465, 260, 0.5, 2.5e5, 54, 4150];
    [TC_feed,RC]=meshgrid(linspace(-18,-10,5),linspace(0.3,0.7,5));
    cost=zeros(1,12);
    for i=1:5
        for j=1:5
            x(1)=TC_feed(i,j);
            cost=[cost;x,cost_function(x,hyCase)];
        end
        x(4)=RC(i,j);
    end

    % figure(2)
    % surf(TC_feed,RC,cost)
    % xlabel('Temperature feed sep')
    % ylabel('Split liquid cold separator')
    % zlabel('Cost')

end

```

D.2 Cost_function.m

Change variables in UnSim and and extract all relevant data.

```
%% Cost_function.m
% Summary:      Insert and exstract data from unisim, can also with small
%               modifications be used as the cost functin in an
%               optimizing algorithm
% author:       Tor Anders Marvik
% organization: Department of Chemical Engineering, NTNU, Norway
% contact:      torandma@stud.ntnu.no
% requires:     matlab and unisim
% todo 1.0:     All the data should advantageously be orgenized in a
%               structure array.
% started      Oktober 2012
%Input:        setpoints to unisim
%Output:       vectores and stucture array with unisim data
%%

function [cost_parameters,merke,c,Temp_profile,data_all] = cost_function(x,hyCase,data_all,i)
stream=hyCase.Flowsheet.MaterialStreams;           %stream path
EnergyStreams=hyCase.Flowsheet.EnergyStreams;      % energy strems
operations=hyCase.Flowsheet.Operations;
col=hyCase.Flowsheet.Operations.Item('21_VE103');
sol=hyCase.Solver;
script_folder='C:\Users\torandma\Documents\prosjekt karsto\matlab';
merke=0;
in=0;

%Setting controller setpoints and other degrees of freedom
sol.canSolve=0;
stream.Item('1b').TemperatureValue=x(1); % C | Temp before feed sep
stream.Item('13').PressureValue=x(2); % kPa | Pressure feed sep
operations.Item('21_PV2001').PressureDrop.Value=x(3); %kPa pressure drop cold sep. - column
RC(1-x(4),script_folder,hyCase) % frac| Split ratio liq. cold sep
EnergyStreams.Item('Q_side_btm').HeatFlowValue=x(5)/3600; %kj/h | energy bmt side boiler
col.ColumnFlowsheet.Specifications.Item('Temperature').GoalValue=x(6); %setpoint column bottom
stream.Item('14').PressureValue=x(7); %kPa |Pressure after expander
stream.Item('D').PressureValue=x(7)-200;
stream.Item('12').PressureValue=x(7)-200; % kPa | Pressure diff cold sep
sol.canSolve=1;

isknown=0; % parameters to check if unisim converges
```

```

isknown=isknown + stream.Item('D').MassFlow.isKnown      -1;
isknown=isknown + stream.Item('B').MassFlow.isKnown      -1;
isknown=isknown + EnergyStreams.Item('E1').HeatFlow.isKnown -1;
isknown=isknown + stream.Item('1').Temperature.IsKnown   -1;
isknown=isknown + stream.Item('1').Temperature.IsKnown   -1;
isknown=isknown + stream.Item('1').Temperature.IsKnown   -1;
isknown=isknown + stream.Item('1b').Temperature.IsKnown  -1;

isknown=isknown + strcmp('Converged',operations.Item('RCY-7').RecycleConvergence) -1;
isknown=isknown + strcmp('Converged',operations.Item('RCY-5').RecycleConvergence) -1;
isknown=isknown + strcmp('Converged',operations.Item('RCY-1').RecycleConvergence) -1;
isknown=isknown + strcmp('Converged',operations.Item('RCY-6').RecycleConvergence) -1;

if isknown<0
    fprintf('Unisim failed to converge\n')
    fprintf('Please solve the problem manually\n\n')
    in = input('Has the problem been solved manually? (y=0/n=1):');
end

if in == 1                                %model not converged, insert zero vector
    cost_parameters=zeros(1,5);
    Temp_profile=zeros(1,39);
    c=zeros(1,8);
    merke=1;
else                                        %model converged, extract data

    %=====cost function parameters=====
    D=stream.Item('D').MassFlowValue*3600;   %kg/h
    B=stream.Item('B').MassFlowValue*3600;   % kg/h
    V=col.ColumnFlowsheet.MaterialStreams.Item('Boilup').MassFlowValue*3600;
    %reboiler energy

    powercomp0=operations.Item('K-100').energyValue*3600; %kJ/h | duty sales gass comp
    powercomp1=operations.Item('K-101').energyValue*3600; %kJ/h | duty sales gass comp
    powercomp2=operations.Item('K-102').energyValue*3600; %kJ/h | duty sales gass comp
    powercomp3=operations.Item('K-103').energyValue*3600; %kJ/h | duty sales gass comp
    powercomp4=operations.Item('K-104').energyValue*3600; %kJ/h | duty sales gass comp
    powercomp5=operations.Item('K-105').energyValue*3600; %kJ/h | duty sales gass comp

    comp_salesgas=powercomp1+powercomp1+powercomp2;
    comp_boster=powercomp3+powercomp4+powercomp5;
    %=====

```

```

%=====constraints=====
c(1,1)=col.ColumnFlowsheet.PressuresValue(end)/100 ;           %[bar] Tower btm pressure
c(1,2)=stream.Item('13').PressureValue/100;                   %[bar] expansion pressure
c(1,3)=col.columnFlowsheet.temperaturesValue(20) ;           %Temperature stage 19
c(1,4)=operations.Item('21_PV2001').PressureDropValue/100;   %[bar] pressure drop column col
c(1,5)=stream.Item('20').TemperatureValue;                   %[C] Temperature befoure compres
c(1,6)=stream.Item('B').componentMolarFractionValue(4);      %methane bottom
c(1,7)=stream.Item('D').componentMolarFractionValue(3);      %CO2 top
c(1,8)=operations.Item('21_HA204').UAValue*3600;            %UA kJ/C*h

Temp_profile=col.columnFlowsheet.TemperaturesValue;

merke=0;
cost_parameters=[D, B, V, comp_salesgas, comp_boster];
%cost=[-1,-2,1,1,1]*cost_parameter,s'; %coment out if the function is to be used
%in the automized optimization

%Creating a struct of all important variables
data_all.constraints.tower_btm_p(:,i)=col.ColumnFlowsheet.PressuresValue(end)/100;
data_all.constraints.expansion_pressure(:,i)=stream.Item('13').PressureValue/100;
data_all.constraints.temp_tray19(:,i)=col.columnFlowsheet.temperaturesValue(20);
data_all.constraints.dela_p_column_coldsep(:,i)=operations.Item('21_PV2001').PressureDropV
data_all.constraints.temp_before_comp(:,i)=stream.Item('20').TemperatureValue;
data_all.constraints.Cl_btm(:,i)=stream.Item('B').componentMolarFractionValue(4);
data_all.constraints.CO2_top(:,i)=stream.Item('D').componentMolarFractionValue(3);
data_all.constraints.UA_21HA204(:,i)=operations.Item('21_HA204').UAValue*3600;

data_all.cost_param.D_flow(:,i)=stream.Item('D').MassFlowValue*3600;
data_all.cost_param.B_flow(:,i)=stream.Item('B').MassFlowValue*3600; % kg/h
data_all.cost_param.V_flow(:,i)=col.ColumnFlowsheet.MaterialStreams.Item('Boilup').MassFlo
data_all.cost_param.compwork_booster(:,i)=comp_boster;
data_all.cost_param.compwork_salesgas(:,i)=comp_salesgas;

%stream data
data_all.feed_sec2=extract_stream_data('feed_sec2',i,stream,data_all.feed_sec2);
data_all.s1=extract_stream_data('1',i,stream,data_all.s1);
data_all.s1b=extract_stream_data('1b',i,stream,data_all.s1b);
data_all.s2=extract_stream_data('2',i,stream,data_all.s2);
data_all.s3=extract_stream_data('3',i,stream,data_all.s3);
data_all.s4=extract_stream_data('4',i,stream,data_all.s4);
data_all.s5=extract_stream_data('5',i,stream,data_all.s5);
data_all.s6=extract_stream_data('6',i,stream,data_all.s6);
data_all.s7=extract_stream_data('7',i,stream,data_all.s7);

```

```

data_all.s8=extract_stream_data('8',i,stream,data_all.s8);
data_all.s9=extract_stream_data('9',i,stream,data_all.s9);
data_all.s10=extract_stream_data('10',i,stream,data_all.s10);
data_all.s11=extract_stream_data('11',i,stream,data_all.s11);
data_all.s12=extract_stream_data('12',i,stream,data_all.s12);
data_all.s13=extract_stream_data('13',i,stream,data_all.s13);
data_all.s14=extract_stream_data('14',i,stream,data_all.s14);
data_all.s15=extract_stream_data('15',i,stream,data_all.s15);
data_all.s16=extract_stream_data('16',i,stream,data_all.s16);
data_all.s17=extract_stream_data('17',i,stream,data_all.s17);
data_all.s18=extract_stream_data('18',i,stream,data_all.s18);
data_all.s19=extract_stream_data('19',i,stream,data_all.s19);
data_all.to_sec7=extract_stream_data('to_sec7',i,stream,data_all.to_sec7);
data_all.D=extract_stream_data('D',i,stream,data_all.D);
data_all.B=extract_stream_data('B',i,stream,data_all.B);
data_all.side_btm_out=extract_stream_data('side_btm_out',i,stream,data_all.side_btm_out);
data_all.side_btm_in=extract_stream_data('side_btm_in',i,stream,data_all.side_btm_in);
data_all.side_top_out=extract_stream_data('side_top_out',i,stream,data_all.side_top_out);
data_all.side_top_in=extract_stream_data('side_top_in',i,stream,data_all.side_top_in);

```

end

end

D.3 Optimaliser.m

The plots was made by the following script

```

%plot of how the different parameters in the cost funtion change
%with one variable

clear all
clc
load('..\TC_col')

cost_parameters=data(2:end,1:5);
x=data(2:end,6:12);
c=data(2:end,13:20);

```

```

temp_profile=data(2:end,20:59);
merke=data(2:end,60);
c_param=[36; 78; -30; 2; -35; 0.01; 0.01; 1.6e6 ]; %c-c_param>=0

p=[-0.39,-1.0,0.022,0.00044,0.00044];

for i=1:length(cost_parameters(:,1))
c_diff(i,1)=-(c(i,1)-c_param(1));
c_diff(i,2)=-(c(i,2)-c_param(2));
c_diff(i,3)=(c(i,3)-c_param(3));
c_diff(i,4)=(c(i,4)-c_param(4));
c_diff(i,5)=-(c(i,5)-c_param(5));
c_diff(i,6)=-(c(i,6)-c_param(6));
c_diff(i,7)=-(c(i,7)-c_param(7));
c_diff(i,8)=-(c(i,8)-c_param(8));

scaled_cost(i,:)=cost_parameters(i,:).*p;
cost(i)=sum(scaled_cost(i,:));
end

x_axis=x(:,6)'
x_label='Temperature col. bottom [*C]';
streng='Infeasible area'

fig=figure(1)
hold on
subplot(4,2,1)
plot(x_axis, ...
      (data_all.cost_param.compwork_booster+data_all.cost_param.compwork_salesgas).*p(4))
%plotting pressure to sec7
xlabel(x_label)
ylabel('Compression cost [NOK/h]')
hold on
plot([x_axis(4) x_axis(4)],get(gca,'YLim'),'r—')
streng='Infeasible area'
text(46,sum(get(gca,'YLim'))/2,streng,'Color','r')
subplot(4,2,2)
plot(x_axis, data_all.cost_param.V_flow.*p(3))
xlabel(x_label)
ylabel('Reboiler cost [NOK/h]')
hold on
plot([x_axis(4) x_axis(4)],get(gca,'YLim'),'r—')

```



```

text(46, sum(get(gca, 'YLim'))/3, streng, 'Color', 'r')

subplot(4,2,3)
plot(x_axis, data_all.cost_param.B_flow.*-p(2))
xlabel(x_label)
ylabel('Income B product [NOK/h]')
hold on
plot([x_axis(4) x_axis(4)], get(gca, 'YLim'), 'r—')
text(46, sum(get(gca, 'YLim'))/2, streng, 'Color', 'r')

subplot(4,2,4)
plot(x_axis, data_all.cost_param.D_flow.*-p(1))
xlabel(x_label)
ylabel('Income D [NOK/h] ')
hold on
plot([x_axis(4) x_axis(4)], get(gca, 'YLim'), 'r—')
text(46, sum(get(gca, 'YLim'))/2, streng, 'Color', 'r')

subplot(4,2,5)
plot(x_axis, data_all.D.x(3, :))
xlabel(x_label)
ylabel('CO2 D [mol frac.]')
hold on
plot([x_axis(4) x_axis(4)], get(gca, 'YLim'), 'r—')
text(46, sum(get(gca, 'YLim'))/2, streng, 'Color', 'r')

subplot(4,2,6)
plot(x_axis, data_all.B.x(4, :))
xlabel(x_label)
ylabel('Methane B [mol frac.]')
hold on
plot([x_axis(4) x_axis(4)], get(gca, 'YLim'), 'r—')
text(46, sum(get(gca, 'YLim'))/2, streng, 'Color', 'r')

subplot(4,2,[7,8])
plot(x_axis, cost')
xlabel(x_label)
ylabel('Total cost [NOK/h]')
hold on
plot([x_axis(4) x_axis(4)], get(gca, 'YLim'), 'r—')
text(46, sum(get(gca, 'YLim'))/2, streng, 'Color', 'r')
%data=[cost_parameters, x, Temp_profile, merke]
%      1:5          6:12      13:51      52

```

```

% c(1,1) Tower btm pressure
% c(1,2) expansion pressure
% c(1,3) Temperature stage 19
% c(1,4) pressure drop column cold sep
% c(1,5) Temperature before compressor
% c(1,6) methane bottom
% c(1,7) CO2 top
% c(1,8) UA kJ/C*h

```

D.4 extract_stream_data.m

Function to make a structure array with data for a specified stream in UniSim

```

function [strom]=extract_stream_data(a,i,stream,strom)

%a is the name of stream
%i is the simulation number

strom.f(:,i)=stream.Item(a).MassFlowValue*3600;
strom.t(:,i)=stream.Item(a).TemperatureValue;
strom.p(:,i)=stream.Item(a).pressureValue/100;
strom.x(:,i)=stream.Item(a).componentMolarFractionValue;
strom.z(:,i)=stream.Item(a).vapourFractionValue;

end

```