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Design configurations of the methanol synthesis loop

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Preface

This master thesis was written in the subject TKP4900, environmental engineering and reactor technology, at the Department of Chemical Engineering (NTNU), in the spring of 2011. The project used Honeywell's general purpose process simulator UniSim Design (R380 Build 14027) combined with MathWorks programming language MATLAB to evaluate different design considerations of the methanol synthesis loop.

Supervisor for the thesis was prof. Magne Hillestad. I greatly appreciate Magne Hillestad for his guidance and good advices during this project.

Kristian Bøhn (Sign.)

Trondheim 11.06.2011

Abstract

In recent years the chemical industry has undergone considerable changes due to increased environmental regulations and energy costs. This master thesis has evaluated three different design considerations of the methanol synthesis loop using Honeywell's general purpose process simulator UniSim Design (R380 Build 14027) combined with MathWorks programming language MATLAB. The three configurations are Lurgis methanol reactor loop as built on Tjeldbergodden, the use of interstage methanol removal by the means of condensation and Lurgis MegaMethanol configuration. It was shown that the base case simulation of Lurgis reactor loop, using kinetics from Vanden Bussche and Froment (1996), gave reasonable results compared to Tjeldbergodden methanol plant.

For the interstage methanol removal configuration it was found that the two reactors should be of equal length, 7.25 m, and that a cooling water temperature of 250°C in the first reactor and 255°C in the second reactor produced the highest amount of methanol. When operating with a recycle ratio of 2, this configuration had the potential of a net present worth of 47 million dollars compared to the base case over a 10 year horizon.

The addition of a gas cooled reactor for the MegaMethanol process only increased the methanol production by 0.2 tonne/h, making the project unfeasible.

Contents

Chapter 1

Introduction

In recent years the chemical industry has undergone considerable changes due to increased environmental regulations and energy costs. Adaptations of both design procedures and operation conditions have been carried out to decrease costs, and to meet regulations. The main goal in plant design has always been to reduce operational and investment cost, while maximising sales income.

Methanol was first isolated by Robert Boyle in 1661 by distillation of boxwood. The first large scale methanol plant was build in Germany by BASF in 1923. The catalyst used in this plant (ZnO/Cr_2O_3) produced methanol at 240-300 bar and 350-400 °C. It also produced by-products like methane and other light hydrocarbons with 2–5 wt.% selectivity (Lange, 2001). More active and selective catalysts were known, but they were not resistant to impurities like sulphur. In the 1960s a major improvement was conducted by the production of a sulphur free synthesis gas. This synthesis gas led to the use of a more active catalyst ($Cu/ZnO/Al_2O_3$), and a new generation of methanol plants called Low-Pressure Plants (50-100 bar and 250-280 °C). The $Cu/ZnO/Al_2O_3$ catalyst, operating at the reduced temperature, has over 99 % selectivity resulting in very little by-product formation (Moulijn et al., 2008).

This thesis uses information based on Tjeldbergodden methanol plant, which started operation June 5th 1997. Tjeldbergodden methanol plant is the largest in Europe, and produces around 900.000 tonnes of methanol each year. The methanol plant receives its raw material (natural gas) from the Heidrun field at Haltenbanken. The volume of methanol produced at Tjeldbergodden equals 25 % of Europe's methanol production, and 13 % of its consumption. Statoil's stake in the plant is 81.7 percent, while ConocoPhillips has the remaining 18.3 percent (Statoil, 2010).

1.1 Design

The methanol synthesis is characterised by the reforming of natural gas to synthesis gas, which is further reacted to methanol. This thesis focuses primarily on the methanol reactor loop, where synthesis gas is used to make methanol. The methanol reactor loop as used on Tjeldbergodden consists of a multitube reactor cooled with boiling water, a heat exchanger, a condenser and a recycle. It is called a loop due to the large recycle stream needed for an acceptable methanol yield and carbon efficiency. Attempts to make a once-through process with e.g. interstage methanol removal by condensation, absorption by a liquid or reactive chromatography have not produced satisfactory results (Lange, 2001).

1.2 Methanol Properties

Methanol (often abbreviated as MeOH) is the simplest alcohol. Methanol at room temperature is a clear, colourless liquid that is both flammable and toxic. It is soluble in water and in most organic solvents. Methanol is generally considered non-corrosive. Its physical data is summarised in Table 1.1. Methanol is solely produced synthetic, and by either of two methods (Aschehoug and Gyldendal, 2006):

- Hydrogenation of carbon monoxide under high pressure in the presence of a catalyst
- Partial oxidation of hydrocarbons from natural gas

Table 1.1: Methanol properties (Methanex, 2010b), (Aylward and Findlay, 2002)

Property	Value	Unit
Freezing point	-97.8	°C
Boiling point	64.7	°C
Critical temperature	239.4	°C
Flash point	11	°C
Auto ignition temperature	385	°C
Vapour pressure	12.8	kPa [20 °C]
Vapour density	1.354	kg m^{-3} [15 °C]
Density	787	kg m^{-3}
Molar mass	32.04	g mol^{-1}
$\Delta_f H^0$ (gas)	-201	kJ mol^{-1}
$\Delta_f G^0$ (gas)	-163	kJ mol^{-1}
$\Delta_{vap} H^0$	38	kJ mol^{-1}
S^0 (gas)	240	J K^{-1} mol^{-1}
C_p^0 (gas)	44	J K^{-1} mol^{-1}
LD_{50}	5628	mg kg^{-1} [oral, rat]

Methanol is primarily used to make other chemical components, but it can also be used as a solvent, as engine fuel and for fuel in fuel cells (Hogarth and Hards, 1996). Formalaldehyde, acetic acid and MTBE are the main chemical components made from methanol. Examples of secondary derivates made from methanol are plywood, particleboard, foams, resins and plastics (Methanex, 2010a).

1.3 Objective

The objective of this project is to find the best configuration of the methanol reactor loop out of three different options. These are:

- Lurgis methanol design as used on Tjeldbergodden.
- Use of methanol removal between the methanol reactors by the means of condensation.
- Lurgis MegaMethanol process.

The first design will serve as the base case for this thesis, and the two other designs will be compared to this.

The reason for studying different design configurations of the methanol synthesis is to increase profit. This can be done by maximizing the methanol yield while minimizing the operational and investment costs. One way of doing this is to simulate the plant and find out if one design has higher or lower profit. For the second process, where methanol is removed by interstage condensation, there are several different operational and design parameters to specify. To find the optimal value for these parameters, one can simulate the process and see what a change in an operational parameter results in. This is done in UniSim by a case study, which will be explained later.

Chapter 2

Theory

2.1 Methanol Production

Methanol is most commonly produced from natural gas. A typical block diagram of such process is shown in Figure 2.1.

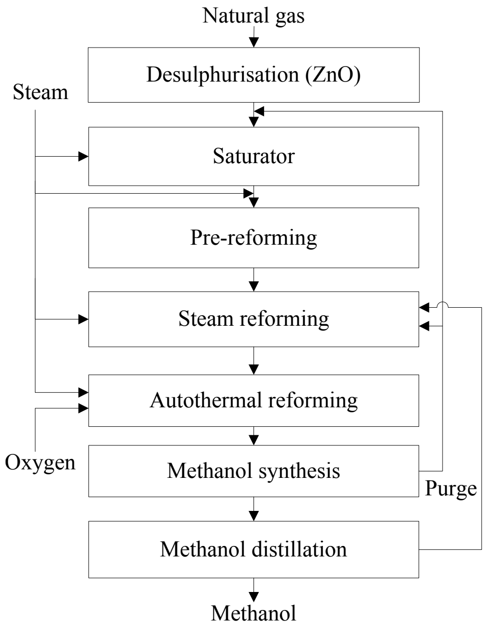

Figure 2.1: Block diagram of a methanol plant

2.1.1 Reforming

The natural gas is first fed to a sulphur removal unit. This is to avoid poisoning of the catalyst used in the following reforming step, which is reforming. Several different reactor layouts can be used for synthesis gas (syngas) production, but today the most common configuration is the combination of a steam reformer and an auto thermal reformer (ATR). This layout is commonly referred to as 'two-step' reforming and is developed by Lurgi and Haldor-Topsøe (Lange, 2001). If the natural gas also contains parts of higher hydrocarbons it is necessary to include a pre-reformer. In the pre-reformer higher hydrocarbons are converted to methane according to Reaction 2.1.

$$C_nH_{2n+2} + \frac{1}{2}(n-1)H_2O \rightarrow \frac{1}{4}(3n+1)CH_4 + \frac{1}{4}(n-1)CO_2 \tag{2.1}$$

Reactions occurring in the reformers are listed below. The steam reformer produces syngas with a stoichiometric number around 3 (Reaction 2.2-2.4), but the gas contains considerable amounts of methane. In the ATR light hydrocarbons are reformed in a mixture of steam and oxygen to achieve close to total conversion of methane. The endothermic reforming duty is provided by the exothermic oxidation reaction happening in the combustion zone of the reactor. The ATR produces syngas with a lower stoichiometric number (Moulijn et al., 2008), which is regulated by the amount of oxygen and steam fed to the ATR.

$$CH_4 + H_2O \rightleftharpoons CO + 3\,H_2 \qquad \Delta H^0_{298} = 206 \text{ kJ/mol} \tag{2.2}$$

$$CO + H_2O \rightleftharpoons CO_2 + H_2 \qquad \Delta H^0_{298} = -41 \text{ kJ/mol} \tag{2.3}$$

$$CH_4 + CO_2 \rightleftharpoons 2\,CO + 2\,H_2 \qquad \Delta H^0_{298} = 247 \text{ kJ/mol} \tag{2.4}$$

$$CH_4 + 1/2\,O_2 \rightarrow CO + 2\,H_2 \qquad \Delta H^0_{298} = -36 \text{ kJ/mol} \tag{2.5}$$

$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O \qquad \Delta H^0_{298} = -803 \text{ kJ/mol} \tag{2.6}$$

$$CO + 1/2\,O_2 \rightarrow CO_2 \qquad \Delta H^0_{298} = -284 \text{ kJ/mol} \tag{2.7}$$

$$H_2 + 1/2\,O_2 \rightarrow H_2O \qquad \Delta H^0_{298} = -242 \text{ kJ/mol} \tag{2.8}$$

In addition to these reactions some coking takes place.

One of the main characteristics of syngas is the stoichiometric number (SN), which is calculated as:

$$SN = \frac{F_{H_2} - F_{CO_2}}{F_{CO} + F_{CO_2}} \tag{2.9}$$

Where F_i is the molar flow of component i. According to the stoichiometry in Reaction 2.17 and 2.18 the ideal theoretical stoichiometric number for methanol production is 2. A small amount of CO_2 (~5%) increases the catalyst activity, so for practical reasons the stoichiometric number for methanol production is slightly higher than 2.

2.1.2 Reactor Loop

As described in Chapter 1 there are three different reactor loop configurations of interest. Lurgis configuration at Tjeldbergodden is shown in Figure 2.2, and involve two reactors in parallel (simulated as one), a heat exchanger, condenser, separator and a recycle. The reactors used are multitube PFR reactors which transfers the heat generated by the reaction to the boiling water outside the tubes (Boiling Water Reactor, BWR). A heat exchanger called the interchanger heats the cold feed stream against the hot product stream from the reactors. This is the same configuration as used at Tjeldbergodden and will serve as a base case for the other methods.

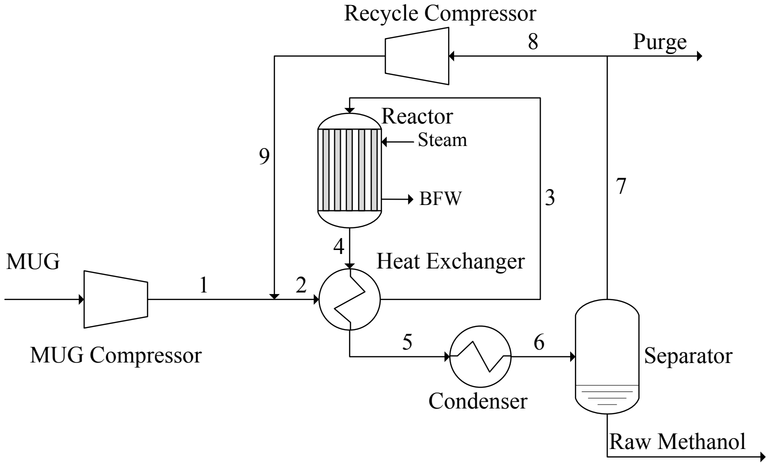

Figure 2.2: The reactor loop

Some of the disadvantages with this configuration is the large recycle stream. This stream has to be recompressed back to the feed pressure resulting in increased compressor duty. It also contributes to larger equipment due to the big gas volume circulating in the loop, and the large volume of gas causes low residence times in the reactors. It was then suggested to set the methanol reactors in series and remove methanol between the reactors by condensation (Figure 2.3). The idea behind this configuration is that the methanol formed in the first reactor is condensed out before entering the second reactor and therefore reducing the volume of the stream entering the second reactor. This will increase the residence time in the second reactor leading to additional methanol production. The disadvantage with this configuration is the extra heating and cooling duty that is needed to condense out the methanol together with the increased pressure drop. The hypothesis is that the advantages of increased methanol production, and the reduced volume of the recycle stream will outweigh the extra duties.

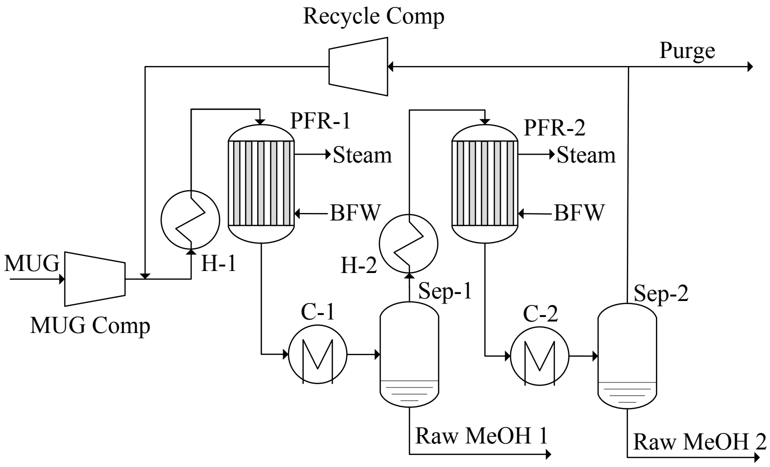

Figure 2.3: PFD of the methanol reactor loop with interstage methanol removal

The MegaMethanol process seen in Figure 2.4 utilised the fact that the methanol reactor and the interchanger are of similar design. Instead of using the interchanger just to transfer heat duty between the feed and product stream, the interchanger is filled with catalyst on the shell side allowing the products from the BWR to continue reacting. The heat generated by the reaction is removed by the counter currant flow of the feed gas to the BWR, and thus called a Gas Cooled Reactor, GCR. In theory this configuration will produce more methanol.

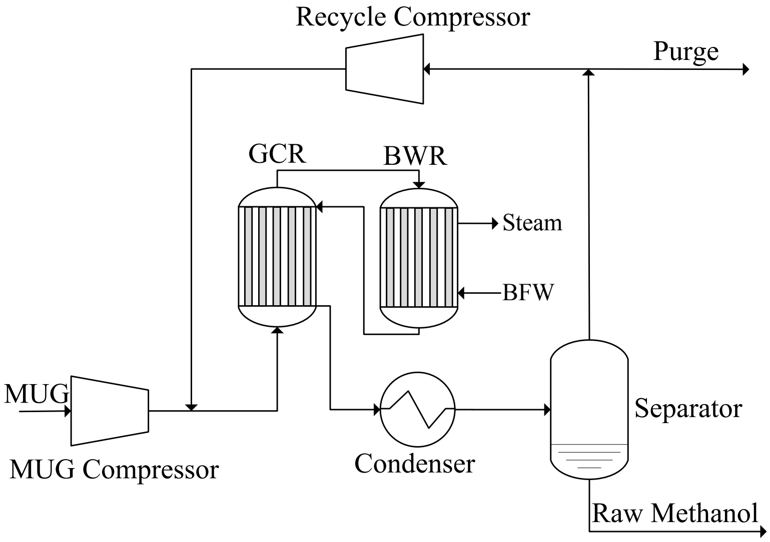

Figure 2.4: MegaMethanol

For other configurations Lange (2001) is recommended.

An important parameter for the reactor loop is the carbon efficiency. The carbon efficiency is a measure of how much of the carbon that enters the loop as CO and CO_2 that leaves the loop as carbon in methanol. The carbon efficiency is therefore an indirect measure of the amount of carbon that is purged. The carbon efficiency is defined as:

$$\text{Carbon Efficiency} = \frac{(F_{\mathrm{CH_3OH}})_{out}}{(F_{\mathrm{CO}} + F_{\mathrm{CO_2}})_{inn}} \tag{2.10}$$

In addition to the carbon efficiency, the recycle ratio is also of importance. The recycle ratio is defined in Equation 2.11.

$$R = \frac{\text{Molar flow in recycle stream}}{\text{Molar flow in feed stream}} \tag{2.11}$$

It can be seen here that the recycle ratio is a parameter showing how large the recycled stream is compared to the feed stream. The recycle ratio has a large influence in many parameters, such as total methanol production, purge flow, inert concentration in the reactor loop and others.

2.2 PFR simulation

The reactors used for methanol production are simulated as a plug flow reactor, PFR, with a catalyst bed. The equations for solving a PFR with constant cooling temperature are given in Equation 2.13-2.15 (Scott Fogler, 2006).

$$\frac{dw}{dV} = \frac{\tilde{R}}{W} \tag{2.12}$$

$$\frac{dT}{dV} = \frac{r_A \Delta H_{rx} - U\frac{4}{D}\left(T - T_c\right)}{W\overline{C_p}} \tag{2.13}$$

$$\frac{dT_c}{dV} = \frac{U\frac{4}{D}\left(T_c - T\right)}{W_c C_{p_c}} \tag{2.14}$$

$$\frac{dP}{dV} = \frac{1.75\rho \left(v'\right)^2}{D_p \psi} \frac{1-\epsilon}{\epsilon^3} A \tag{2.15}$$

Equation 2.15 is the turbulent part of Erguns equation, which calculates pressure drop through packed beds.

As described above, the GCR is cooled by a counter current flow of cold syngas. Since UniSim is only able to utilise co-current cooling of the PFR, the simulation of the GCR had to be done in MATLAB. The situation for a countercurrent cooled reactor is that both inlet temperatures are known, but neither of the outlet temperatures. To solve this two point boundary value problem, orthogonal collocation in MATLAB was used (Eaton, 1997). The method of orthogonal collocation is to divide the reactor into 2 boundary condition points, and n internal collocation points. Each collocation point is represented as a residual that are to be zero. The chosen independent variable, in this case the reactor volume, must be normalized:

$$\xi = \frac{V}{V_{tot}}$$

The solution in each internal point is calculated by the Lagrange polynomial:

$$y\left(\xi\right) = \sum_{i=0}^{n} y_i \varphi_i\left(\xi\right)$$

$$\varphi_i\left(\xi\right) = \prod_{k=0,k\neq i}^{n} \frac{\left(\xi - \xi_k\right)}{\left(\xi_i - \xi_k\right)}$$

The orthogonal collocation method also yields discrete approximations to differential operators:

$$\left(\frac{dy}{d\xi}\right)_{\xi_i} = \sum_j A_{i,j} y_j$$

To force the residuals to zero, MATLABs optimizer fsolve is used. Fsolve solves a system of nonlinear equation by finding the root (zero) of the problem. The problem must be specified by:

$$F(x) = 0 \tag{2.16}$$

Where x is a vector and $F(x)$ is a function that returns a vector value (MathWorks, 2011).

2.3 Reaction Kinetics

Independent of the reactor loop configurations, the reactions occurring in any of the methanol reactors are:

$$CO + 2\,H_2 \rightleftharpoons CH_3OH \qquad \Delta H^0_{298} = -90.8 \text{ kJ/mol} \tag{2.17}$$

$$CO_2 + H_2 \rightleftharpoons CO + H_2O \qquad \Delta H^0_{298} = 41 \text{ kJ/mol} \tag{2.18}$$

$$CO_2 + 3\,H_2 \rightleftharpoons CH_3OH + H_2O \qquad \Delta H^0_{298} = -49.6 \text{ kJ/mol} \tag{2.19}$$

Out of the three reactions above, only two are independent. Reaction 2.17 is the hydrogenation of CO, Reaction 2.18 is the reverse water gas shift reaction (RWGS) and Reaction 2.19 is the hydrogenation of CO_2. The conversion of CO and CO_2 at equilibrium is shown in Table 2.1. As seen in this table, and since the methanol reactions are exothermic, low temperatures are favourable (the CO_2 conversion increases with temperature due to the reverse water gas shift reaction).

Table 2.1: Equilibrium data for CO and CO_2 conversion (Moulijn et al., 2008)

	CO conversion			CO_2 conversion		
Temp [°C]	Pressure [bar]			Pressure [bar]		
	50	100	300	50	100	300
252	0.524	0.769	0.951	0.035	0.052	0.189
302	0.174	0.440	0.825	0.064	0.081	0.187
352	0.027	0.145	0.600	0.100	0.127	0.223
402	0.015	0.017	0.310	0.168	0.186	0.260

The rates of the reactions occurring in the methanol reactor are found from both Graaf et al. (1988) and Vanden Bussche and Froment (1996). The main difference between these two articles is which of the reactants that serves as carbon source for the methanol formation. Graaf et al. (1988) compares previously published articles, and concludes that the safest way is to include both CO and CO_2 as the source, while Vanden Bussche and Froment (1996) only includes CO_2. The reason for this is studies performed with labelled C^{14} isotopes which Vanden Bussche and Froment (1996) used to eliminate CO as a carbon source. Based on previous simulations where kinetics from Graaf and Vanden Bussche were used, it was concluded that Vanden Bussche kinetics describes the methanol production best and is thus used in this thesis. The kinetics from Vanden Bussche and Froment (1996) is tested at pressures up to 50 bar, but it is assumed that it provides acceptable results at 80 bar.

These reaction rates are developed using a fresh, pulverized catalyst, and in a bench scale set up. When simulating a large industrial reactor with catalyst pellets, one has to take account for the activity of the catalyst, a, and the internal effectiveness factor, η. The correlation between the reaction rate, activity and effectiveness factor is given in Equation 2.20.

$$r_{Actual}(t) = a(t) \cdot \eta \cdot r \tag{2.20}$$

2.3.1 Activity

The activity of the catalyst is 1 when the catalyst is fresh, but deactivates over time as a result of sintering (aging), fouling and poisoning (Scott Fogler, 2006). The activity is defined as:

$$a\left(t\right) = \frac{r\left(t\right)}{r\left(t=0\right)} \tag{2.21}$$

As indicated by Equation 2.21, the activity of the catalyst is decreasing over time. A common way to counteract this phenomenon is to increase the temperature, or the pressure. The temperature must not exceed the operating temperature of the catalyst, (∼300 °C) because at this temperature unacceptable sintering of the catalyst will take place (Ertl et al., 1997). For the new MK-121 methanol catalyst from Haldor-Topsøe the operating temperature is between 200-310 °C (Haldor-Topsøe, 2011). It is assumed that the catalyst used in this thesis is fresh.

2.3.2 Internal Effectiveness Factor

The effectiveness factor has a magnitude ranging from 0 to 1, and implies the relative importance of diffusion and reaction limitations inside the catalyst pellet (Scott Fogler, 2006). The internal effectiveness factor is defined as

$$\eta = \frac{\text{Actual overall rate of reaction}}{\begin{array}{l}\text{Rate of reaction that would result if entire interior surface were} \\ \text{exposed to the external pellet surface conditions}\end{array}}$$

And is in symbols described as

$$\eta = \frac{-r}{-r_s}$$

Where the subscript s indicates the reaction rate evaluated at the surface conditions.

The internal efficiency factor is greatly dependent on the dimensions of the catalyst particle. Smaller particles will have a larger factor but also create a larger pressure drop through the reactor, due to the more dense packing. The efficiency factor is assumed to be the same for all of the reactions that takes place in the methanol reactor. Hillestad (1995) performed a simulation of the internal effectiveness factor for the catalyst used in methanol synthesis, and found that η would typically have a value of 0.7.

Chapter 3

Simulation of Different Reactor Loop Configurations

The three different reactor loop configurations described in Chapter 2.1.2 where simulated. Lurgis methanol synthesis as built on Tjeldbergodden served as the base case.

3.1 Base Case

Lurgis methanol reactor loop was simulated using Honeywell's process simulator UniSim. Peng-Robinson was selected as the property package for the simulation because it is a well known package, and has been enhanced to yield accurate phase equilibrium calculations for systems containing CH_3OH. The SRK property package would be the second choice, but this package should not be used for systems including CH_3OH (Aspen Technology, 2005). A sketch of the base case is given in Figure 2.2.

The make up gas (MUG) composition is meant to resemble the conditions at Tjeldbergodden methanol plant and is given in Table 3.1.

Table 3.1: Make up gas composition

Component	Molar flow [kmol h^{-1}]	Composition [mol%]
CO	2377	21
CO_2	931	8.2
H_2	7825	69.1
H_2O	10	0.1
CH_3OH	0	0
CH_4	180	1.6
Total	11323	100

The MUG enters the loop at 25°C and 30 bar. It is compressed to 80.3 bar, and mixed with the recycle stream. This stream enters the tube side of the interchanger, where it is heated against the hot products from the reactor. The heat exchanger has a specified cold outlet temperature of 210°C, and a pressure drop of 0.3 bar on each side (Appendix A). The reactor is a multitube PFR with the catalyst pellet inside the tubes. The reactor specifications and the catalyst specifications are given in Table 3.2.

Table 3.2: PFR specifications

	Parameter	Value	Unit
Design	Tube length	7.25	m
	Number of tubes	11030	
	Wall thickness	0.002	m
	Total volume	103	m^3
Cooling	Heat transfer coefficient	1000	$W\ m^{-2}\ °C^{-1}$
	Mole flow	10^{20} [1]	$kmol\ h^{-1}$
	Heat capacity	870000	$J\ mol^{-1}\ °C^{-1}$
	Inlet temperature	250	°C
Catalyst	Particle diameter	0.006	m
	Particle sphericity	0.857	
	Solid density	1950	$kg\ m^{-3}$
	Bulk density	1170	$kg\ m^{-3}$
	Solid heat capacity	250000	$kJ\ kg^{-1}\ °C^{-1}$
	Void fraction	0.40	

The reactor and the catalyst information are collected from the already constructed reactor at Tjeldbergodden (Hillestad, 1995; Haldor-Topsøe, 2011). The boiling water used as a cooling medium will have the same inlet and outlet temperature of 250°C. This is achieved by simulating the cooling medium with a large flow of water (See [1] in Table 3.2).

The interchanger does not provide sufficient cooling duty to condense out the methanol, so this is done in a separate condenser. The condenser has a specified pressure drop of 0.2 bar and an outlet temperature specified to 20 °C. The methanol and water is separated from the recycle stream in a gas-liquid separator, and sent to a temporary storage tank. The stream leaving the top of the separator is split into a purge stream and a recycle stream, where the recycle stream is recompressed back to the feed pressure of 80.3 bar. The reaction set associated with the PFR is given in Appendix B.

3.2 Interstage Methanol Removal

The simulation basis used for the base case was also used for this simulation. The layout of the heat exchanger network was constructed using pinch technology (4.2.5).

After the MUG stream and the recycle stream are mixed it enters the shell side of a heat exchanger. On the tube side the hot products from the second PFR heats the feed to the first PFR. The heat exchanger has a pressure drop of 0.2 bar on each side (See Appendix A), and a specified cold stream outlet temperature of 210 °C. The PFR reactors are constructed with the same specifications as the one in the base case (Table 3.2) except that the number of tubes in each PFR is 5515. The products leaving the first reactor are cooled in a heat exchanger against the cold gas leaving the first separator. The heat exchanger has a pressure drop of 0.2 bar on each side, and a specified outlet temperature of 240 °C. The heat exchanger does not have sufficient cooling to condense out the methanol, so an additional condenser is placed between the heat exchanger and the separator. The condenser uses cooling water at 15 °C and has a specified hot product outlet temperature of 30 °C. After the gas leaves the separator it is reheated in the heat exchanger, and sent to the second PFR. The products from the second PFR are cooled in the first heat exchanger. The gas is passed through another condenser similar to the first, where methanol and water is removed. The gas leaving the second separator is split into a purge stream and a recycle stream. The recycle stream is recompressed, and mixed with the MUG stream.

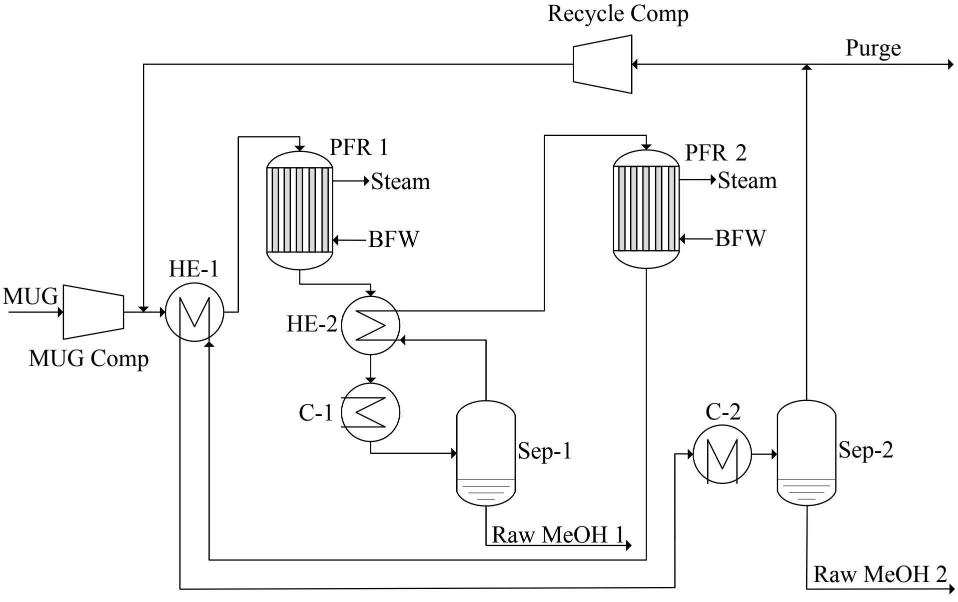

Figure 3.1: Interstage methanol removal

3.3 MegaMethanol

The already built interchanger at Tjeldbergodden was used as basis for the GCR. The design specifications for the interchanger are shown in Table 3.3.

Table 3.3: GCR specifications

Parameter	Value	Unit
Length	18	m
Tubes	5412	
Inner diameter	19	mm
Shell diameter	2.50	m
Heat transfer coefficient	150	$\mathrm{W\ m^{-2}\ °C^{-1}}$
Tube volume	27	$\mathrm{m^3}$
Shell volume	24	$\mathrm{m^3}$

The gas cooled reactor used in the MegaMethanol system was not possible to simulate in UniSim due to the limitation to co currant cooling. It was therefore simulated using Mathworks computing software MATLAB. To be able to simulate the process in MATLAB some assumptions were made. These assumptions are:

- The heat of reaction is independent upon temperature.
- Fugacity coefficients for the components are equal to 1.
- Constant component heat capacities.
- No pressure drop in the GCR.

The three first assumptions are shown to be valid in Hillestad (1995). The assumption of no pressure drop in the GCR was made to make it simpler to solve the GCR. The pressure drop would only have negligible impact on the methanol production.

First it was important to see that MATLAB and UniSim produce the same results. Inlet values from the base case BWR in UniSim was implemented in a MATLAB script, and values calculated by both MATLAB and UniSim were compared. To simulate the BWR, MATLABs ODE45 solver was used. The scripts made to do this can be found in Appendix C.

The next step in simulating the process was to use MATLAB to open an interface between itself and UniSim, so that MATLAB could read information from UniSim, and write the calculated values back. Since this is a reactor loop MATLAB would also have to handle the recycle iteration. The commands written in Table 3.4 opens a ActiveX/COM interface between MATLAB and UniSim, allowing MATLAB to retrieve information from the simulation run in UniSim.

Table 3.4: Commands to open MATLAB/UniSim interface

`h= actxserver('UnisimDesign.Application')`	Creates an ActiveX server
`hyCase= h.Activedocument`	Call the active simulation
`f= hyCase.Flowsheet`	Call the current flowsheet
`g= f.MaterialStreams`	Call a material stream
`sol= hyCase.Solver`	Call the UniSim solver
`sol.CanSolve = 1`	Turn on the UniSim solver

To get the temperature in stream 2 one would have to write everything in Table 3.4 and then "g.Item('2').TemperatureValue".

The script for simulating the MegaMethanol process was then developed step by step. First the GCR was modelled, without the recycle, using orthogonal collocation as described in Chapter 2.2. Then the recycle iteration was modelled. The recycle was modelled by a fsolve where the component mass flows, pressure and temperature at point 2' in Figure 3.2 were guessed, without the GCR, and comparing these to the values in 2 after calculating the BWR and returning the values to UniSim. This way UniSim does all the thermo dynamical calculations, but the recycle and BWR are lifted out to MATLAB. Finally these scripts were combined. In the MegaMethanol script fsolve has to guess the values at 2' and 4 to solve the GCR and BWR simultaneously. The MATLAB script for simulating the MegaMethanol process can be found in Appendix E.

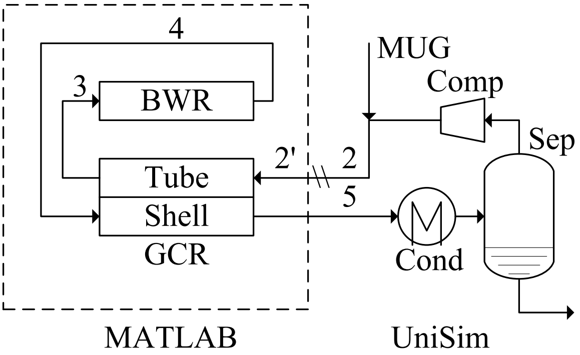

Figure 3.2: Sketch of the MegaMethanol process

Chapter 4

Results and Discussion

The simulations were constructed as explained in Chapter 3. All results were generated using kinetics from Vanden Bussche and Froment (1996) with $a\eta$ equal to 0.7. The compressors used had an adiabatic efficiency of 85 %.

4.1 Base Case

The base case was simulated as described in Chapter 3.1. The base case represents the standard, which the other designs will be compared against, since this configuration is well known and is currently in use by Statoil at Tjeldbergodden. The setup of the simulation is presented in Figure 4.1. The temperature profile and weight fractions in the PFR are presented in Figure 4.2 and 4.1. Data generated from the simulation can be found in Appendix G. Key results are presented in Table 4.1

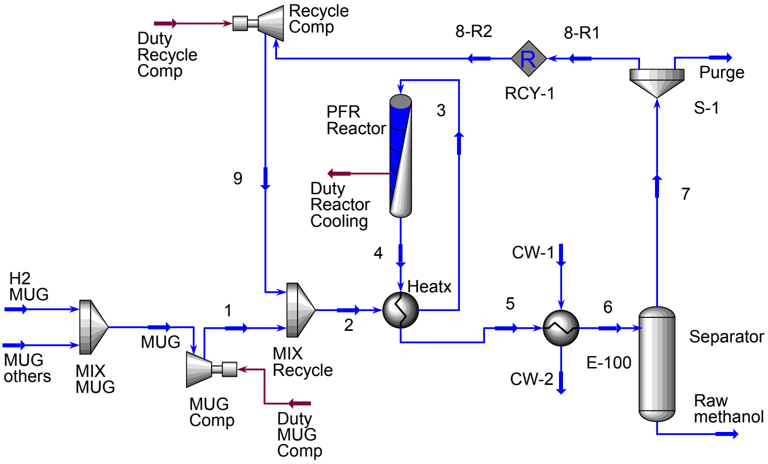

Figure 4.1: Temperature profile in the base case PFR

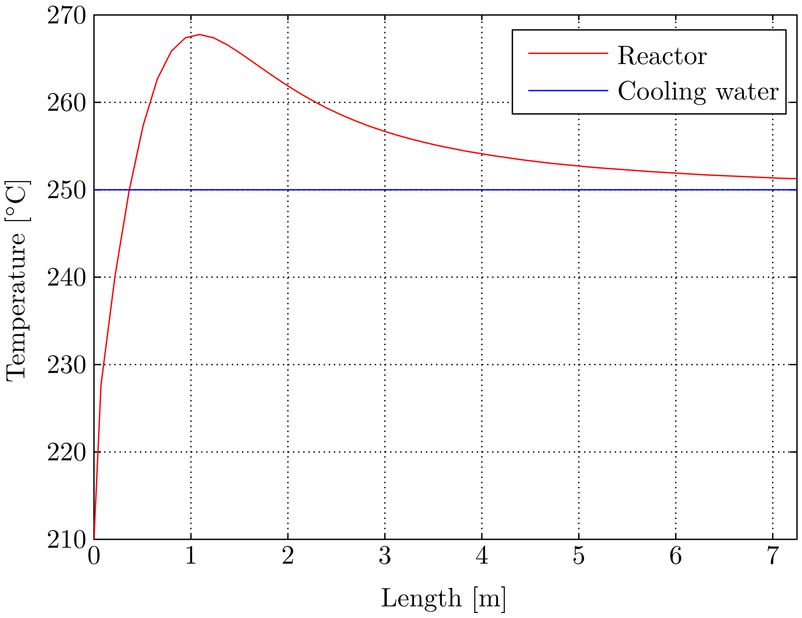

Figure 4.2: Weight fractions in the base case PFR

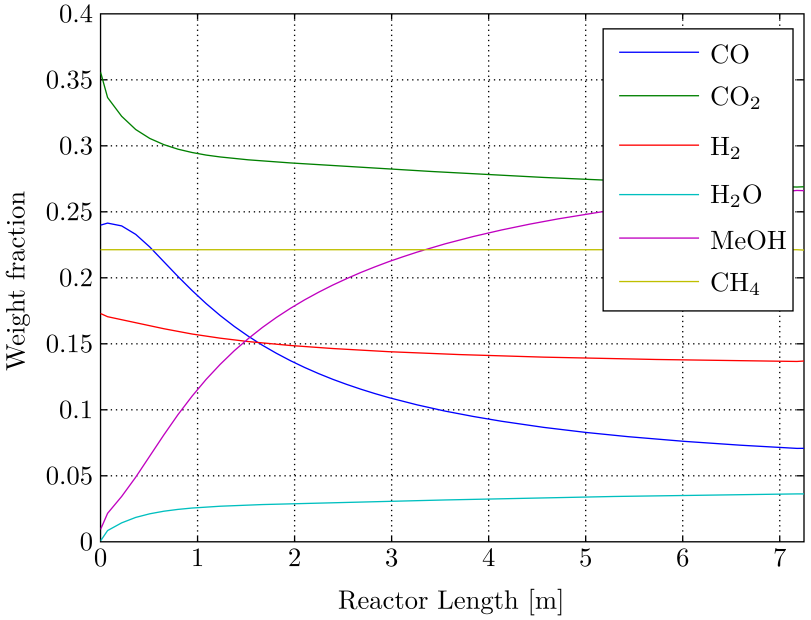

Figure 4.3: Base case simulation

Table 4.1: Key values from the base case simulation

Variable	Value	Unit
SN	2.08	-
Recycle ratio	3	-
Recycle power	572	kW
Inert concentration	11.83	%
Carbon efficiency	94.06	%
Methanol production	3 112	kmol h^{-1}
Purge flow	1 076	kmol h^{-1}
Purge energy	378	GJ h^{-1}
MP steam production	127	tonne h^{-1}

To find the energy of the purge stream, a Gibbs reactor was connected to the purge. The Gibbs reactor minimizes the Gibbs free energy, so when oxygen was sent into the reactor the reactive components in the purge stream, CO,H_2,CH_3OH and CH_4, were reacted to CO_2 and H_2O. The temperature in the outlet stream was set so there were no liquids present. The medium pressure steam production was calculated by routing the energy from the reactor into a heater. The inlet stream was water at 250 °C with a vapour fraction of 0, while the outlet stream was specified with 250 °C and a vapour fraction of 1.

A methanol production of 3112 kmol/h corresponds to approximately 800 000 tonnes annually with the assumption of 8000 working hours per year. In Chapter 1 it is stated that Tjeldbergodden produces 900 000 tonnes annually. The reason for this deviation can be a slightly different reactor layout, more than 8000 working hours, fluctuations in the MUG stream or imperfections in the simulation kinetics.

4.2 Interstage Methanol Removal

The same simulation basis as in the base case was used in this simulation. Several case studies were performed with the system simulated in UniSim. A case study in UniSim varies a chosen parameter, while tabulating the response in the parameters of interest. The only difference between the base case and the case study is the chosen variable. All other inputs are kept constant, if not otherwise specified. The simulation is shown in Figure 4.4, and data from the simulation can be found in Appendix F.

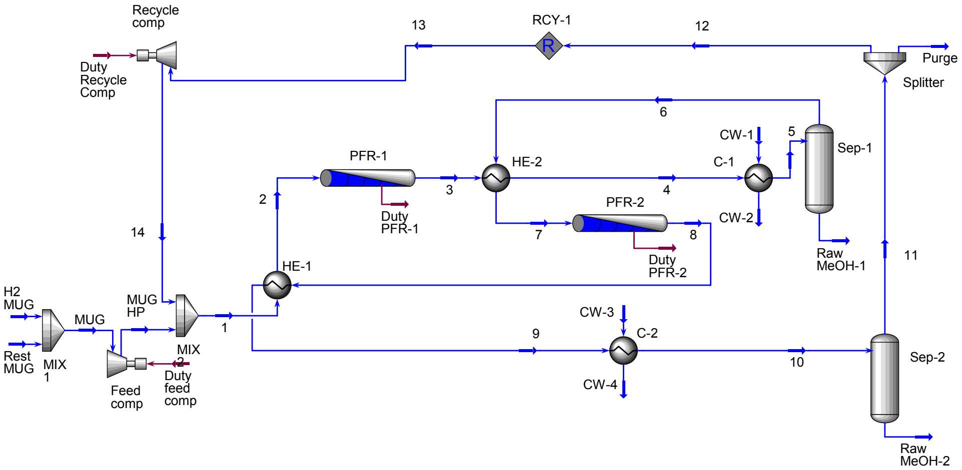

Figure 4.4: Interstage methanol removal simulation

4.2.1 Length

One of the first encountered design issues with the new design was the individual length of the two reactors. The reactors used in the base case have an individual length of 7.25 m, but these are set parallel to each other. If the reactors are placed in series instead the first reactor will have a larger volume flow than the second, due to methanol and water are removed in between, and it may be beneficiary with a shorter reactor first. A case study was conducted where the length of the first reactor was changed. The length of the second reactor was set to 14.5 m minus the length of the first reactor. Both methanol production and pressure drop was recorded, and the results are shown in Figure 4.5.

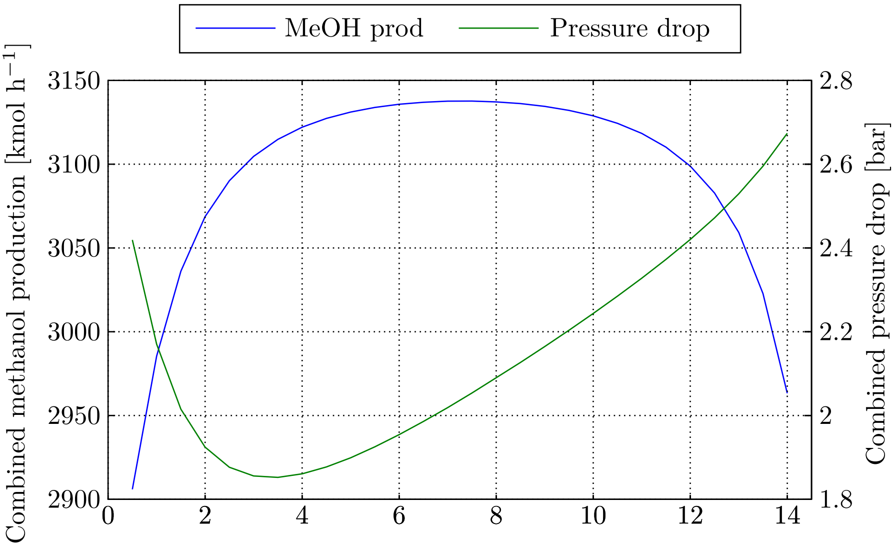

Figure 4.5: Length of the first PFR

From Figure 4.5 it can be conducted that a configuration where both of the reactors are of equal length yields the largest methanol production. On the other hand the combined reactor pressure drop is lowest when the first reactor is shorter than the second, due to the higher gas velocity in the first reactor. It is desirable to build two identical reactors rather than two with different length due to the decreased construction cost. Since the difference in pressure drop at the minimum and where the two reactors are of the same length is less than 0.2 bar it is likely that the reactors should be constructed with the same length.

4.2.2 Cooling Water Temperature

As explained in Chapter 2.1.2 low temperatures are favourable for high equilibrium conversion, however higher temperatures are needed for larger reaction rates. To find the optimum operating temperatures, a case study varied the cooling water temperatures, and the resulting methanol production was recorded. The resulting contour plot is shown in Figure 4.6.

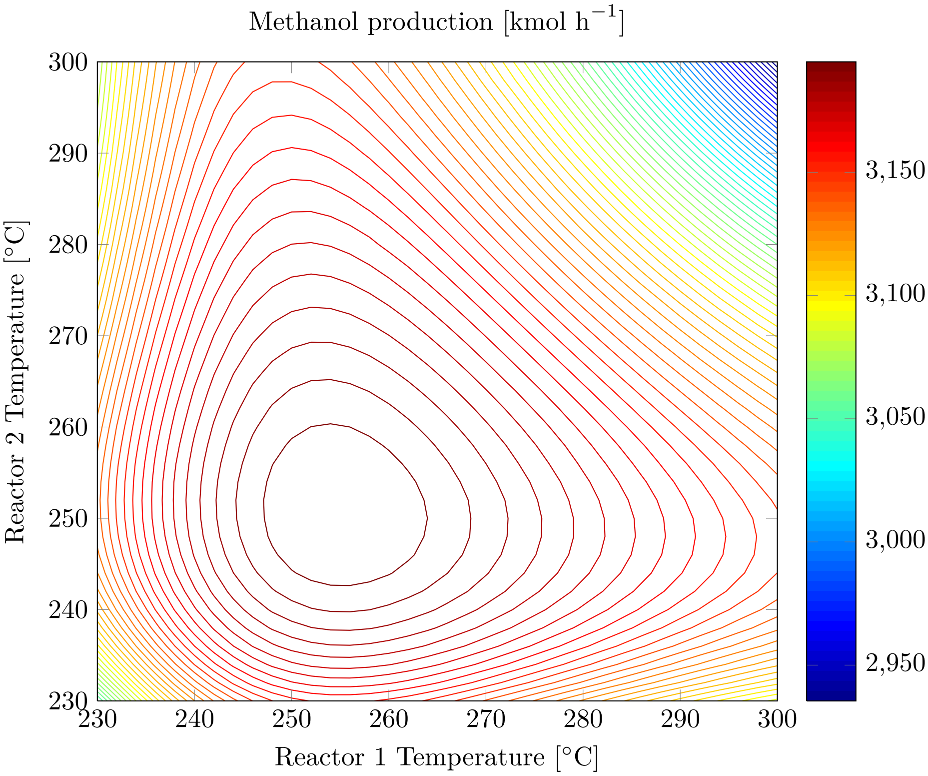

Figure 4.6: Methanol production at different cooling water temperatures

Figure 4.6 shows that the maximum methanol production is attained when the temperature in the first PFR is between 245 and 265°C and between 240 and 260°C in the second. The area between these temperatures is a bit flat, making the highest methanol production hard to find. A closer view of this area is found in Figure 4.7

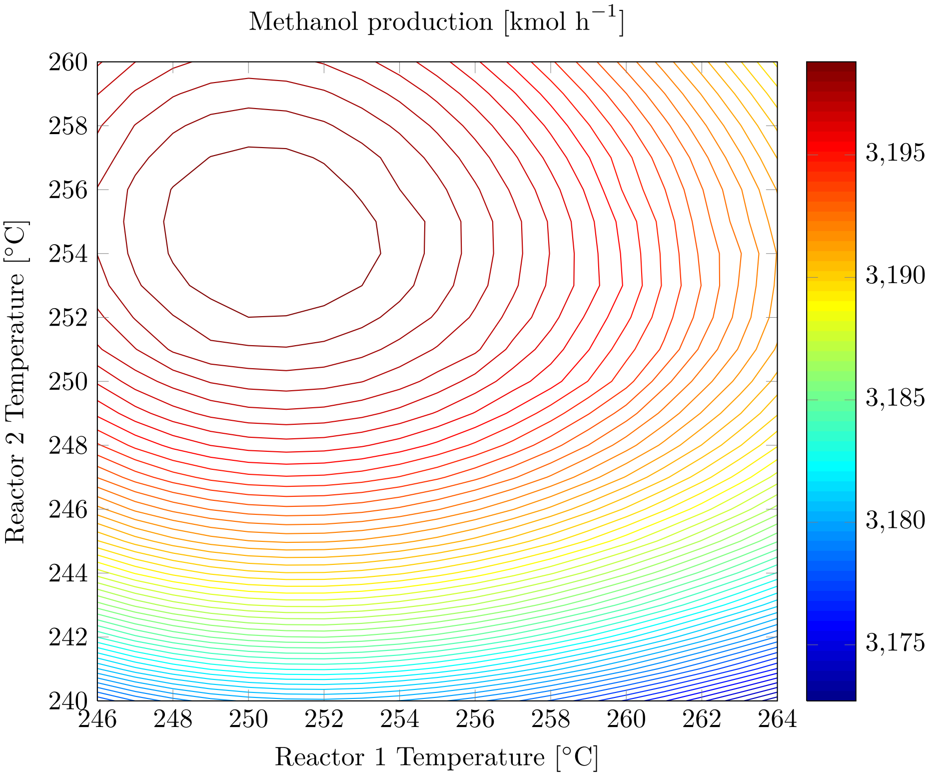

Figure 4.7: Close up of Figure 4.6

In Figure 4.7 it is shown that the optimum cooling water temperature is 250°C in the first reactor and 255°C in the second reactor. As explained in Chapter 2.3.1 the temperature in the reactor must never exceed 300°C because of unacceptable sintering of the catalyst. As Figure 4.8 shows, the highest temperature in the reactor is about 10–15°C above the cooling water temperature, resulting in a max temperature of about 265°C in the reactor when the cooling water temperature is around 250°C.

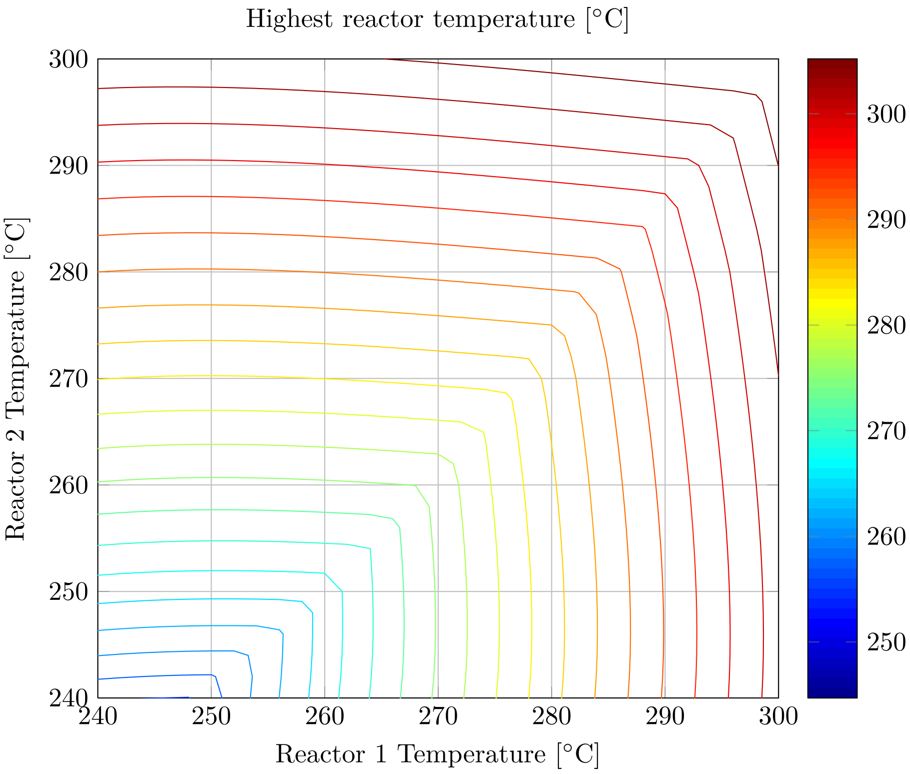

Figure 4.8: Cooling water temperatures and reactor temperatures

4.2.3 Recycle Ratio

Increasing the recycle ratio to achieve an increased methanol production is an important operational parameter. The recycle is limited by the cost of recompressing the recycle stream, and the cost of larger equipment due to the increased gas volume in the loop. The previous figures where all made with a recycle ratio equal to 2. To check if this value is appropriate a new case study was made. The results of this study are viewed in Figure 4.9 and Figure 4.10.

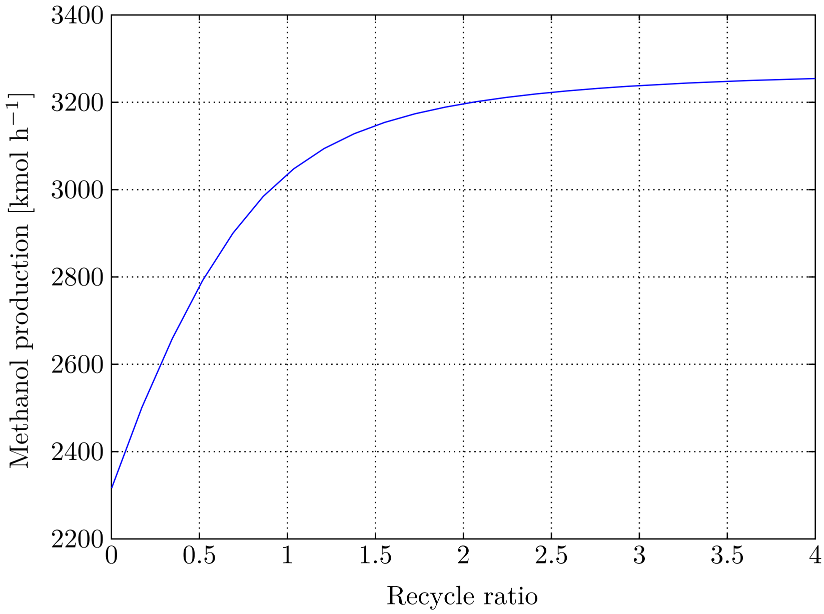

Figure 4.9: Methanol production

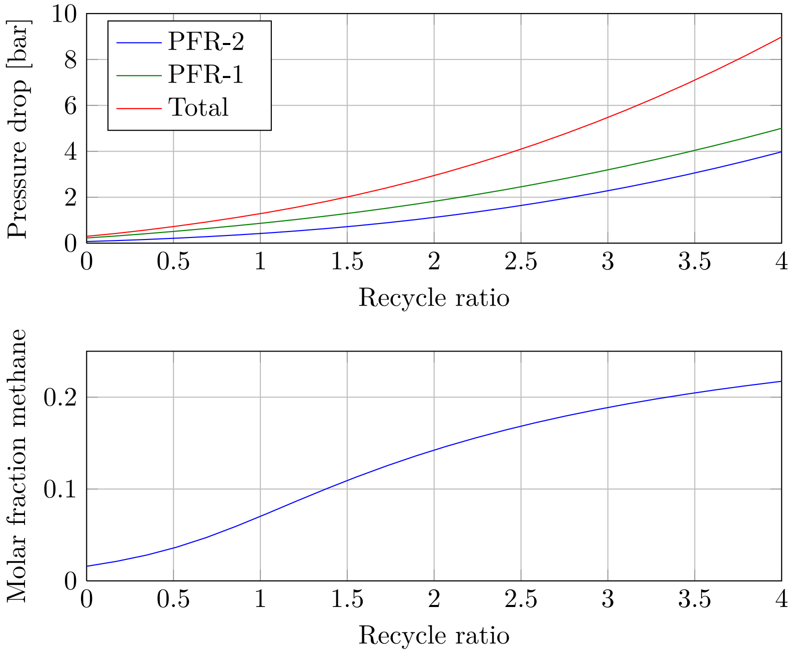

Figure 4.10: Inert concentration and pressure drop

Considering that Figure 4.9 and Figure 4.10 does not have a maximum point it can be difficult to find the ideal recycle ratio. Considering this a recycle ratio of 2 seems reasonable.

4.2.4 Economic Comparison With Base Case

Some key values from the two simulations are given in Table 4.2.

Table 4.2: Comparison of key values from the methanol removal and base case configuration

Variable	Base Case	Interstage removal	Change	Unit
Recycle ratio	3.0	2	-33 %	-
Recycle power	572	997	74 %	kW
Inert concentration	11.83	14.36	21 %	%
Carbon efficiency	94.06	96.71	3 %	%
Methanol production	3 112	3 199	3 %	kmol h^{-1}
Methanol production	99.71	102.51	3 %	tonne h^{-1}
Purge flow	1 076	770	-28 %	kmol h^{-1}
Purge energy	378	292	-23 %	GJ h^{-1}
MP steam production	127	129	2 %	tonne h^{-1}

From Table 4.2 it is clear that the interstage methanol removal configuration produce a greater amount of methanol. To find out if this increase in production is enough to compensate for the extra investment and recycle cost, an economical analysis was made. This analysis compares the difference in investment cost, operating cost and income between the base case and the interstage methanol removal configuration. This difference is used in a rentability study where the net present worth and the discounted cash flow rate of return are calculated. It is assumed that there are no extra operational problems for the interstage configuration due to the similarity with the base case. Trends produced from the rentability analysis are viewed in Figure 4.11, and key values from the economy comparison are listed in Table 4.3. Both analysis were done in Microsoft Excel and can be found in Appendix I.

Table 4.3: Key values from the economy comparison

	Base Case	Two PFR	Difference	Unit
Investment cost	8 400 000	12 340 000	3 940 000	$
Operating cost	180 000	310 000	130 000	$ $year^{-1}$
Income	387 360 000	396 520 000	9 160 000	$ $year^{-1}$

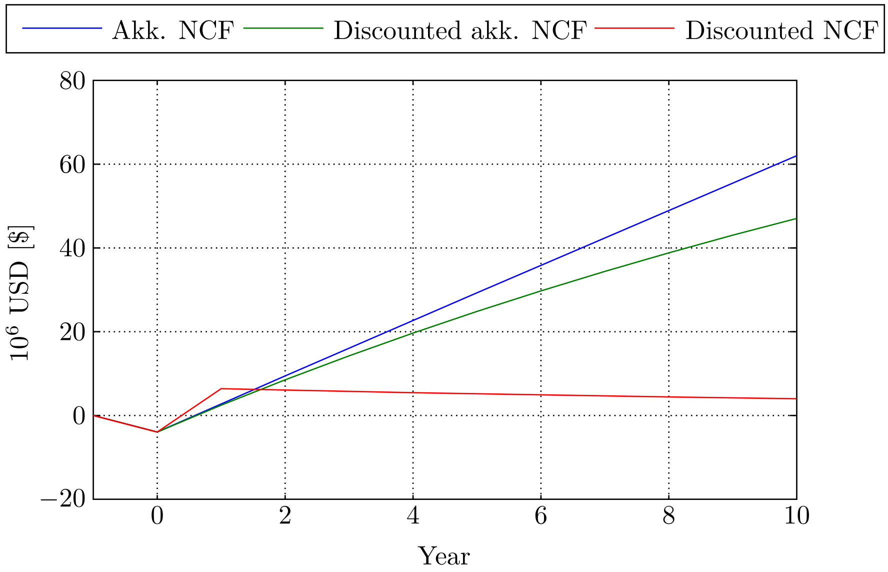

Figure 4.11: Interstage methanol removal cash flow

Table 4.4: Important economic parameters

Parameter	Value	Unit
Rate of return (ROR)	229	%
Discounted cash-flow ROR	170	%
Net present worth (NPW)	47 055 000	$
Payback time	0.5	Years
Project horizon	10	Years

From Table 4.3 it is shown that the increased methanol production yields over 9 million dollars each year, and the investment cost difference is only approximately 4 million dollars. This clearly shows that the increased investment cost for the interstage methanol removal configuration is recouped before a year has passed. This is also viewed in Figure 4.11 as the intersection between the x-axis and the net cash flow line. Table 4.4 presents results of the analysis and predicts a net present worth of over 47 million dollars over a 10 year horizon.

The numbers produced from the economical analysis can be very sensitive in certain parameters. To find out which, a sensitivity analysis was made. This analysis changes the value of a parameter by a specified percentage, and plots the resulting response in the net present worth of the project. The result from the analysis can be seen in Figure 4.12

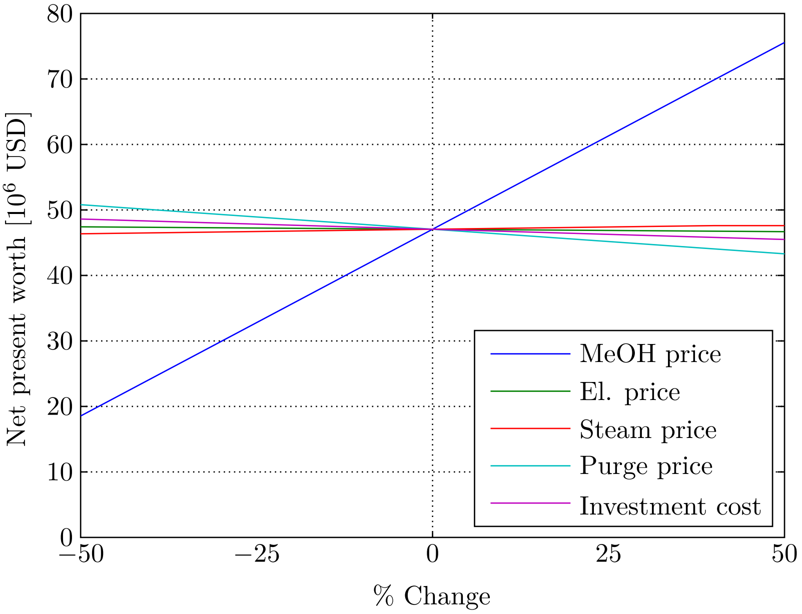

Figure 4.12: Sensitivity analysis

It is shown in Figure 4.12 that the methanol price has the largest influence on the net present worth of the project. Still, a 50 % reduction in the methanol price yields slightly below 20 MUSD in NPW over a 10 year horizon. Other parameters like investment cost, el. price, purge and steam price have little influence in the net present worth.

4.2.5 Pinch Analysis

To find the optimum configuration for the heat exchanger network, a pinch analysis was conducted (Gundersen, 2001). A pinch analysis is based on composite curves for the hot and cold streams in the facility, and uses these to find the pinch point in the process. The data was extracted from the simulation shown in Figure 4.13. The results from this analysis is found in Figure 4.14 and in Appendix 4.2.5.

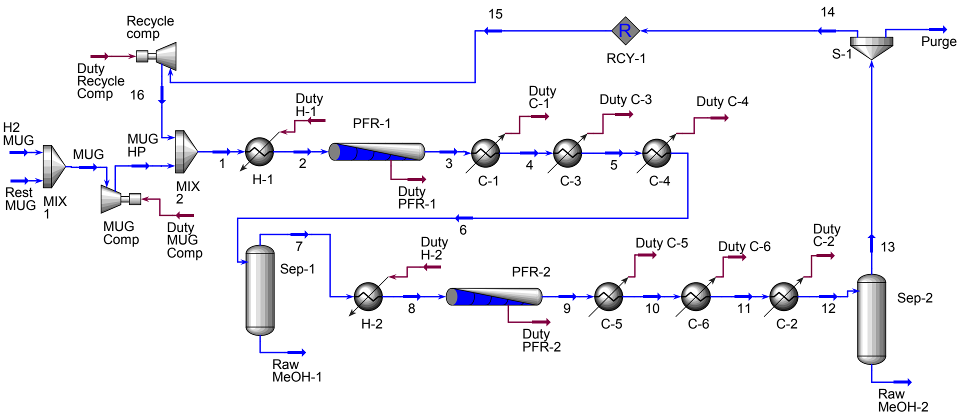

Figure 4.13: UniSim layout

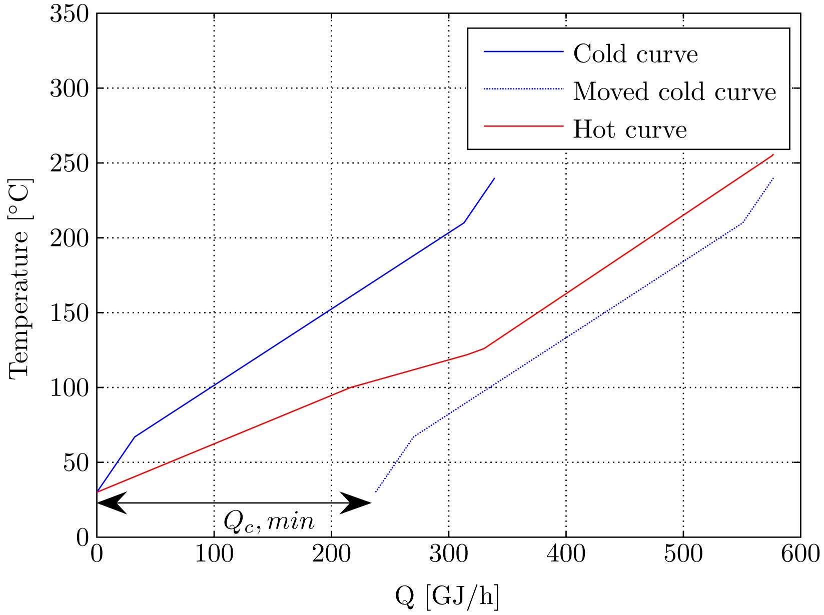

Figure 4.14: Composite curves

In Figure 4.14 it is shown that the pinch point is at the top of the graph. This means that it is not possible to transfer energy through the pinch point, and that ΔT_{min} is equal to the temperature difference at the top of the curve. ΔT_{min} is then equal to

$$\Delta T_{min} = (256 - 240)^\circ\text{C} = 16^\circ\text{C} \tag{4.1}$$

The design criteria below the pinch point is

$$mCp_H \geq mCp_C \tag{4.2}$$
$$n_H \geq n_C \tag{4.3}$$

Where n is the number of hot and cold streams. Since the criteria in Equation 4.3 were valid for both possible heat exchanger configurations, the heat exchanger network with the least total heat exchanging area would be the best. The two possible configurations were both tested in UniSim, and the optimal network is shown in Figure 4.15 and Figure 3.1.

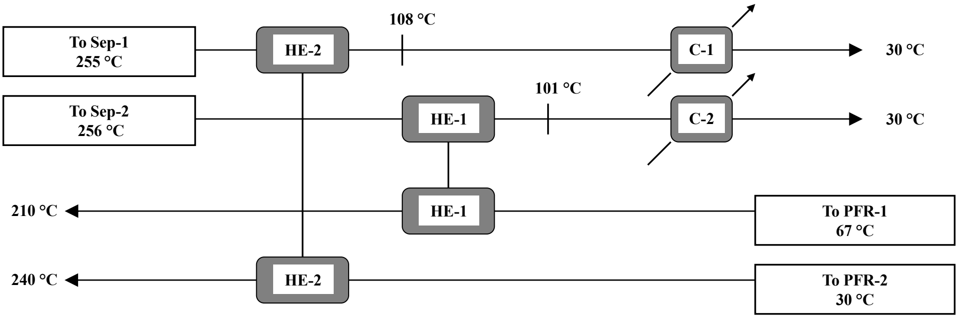

Figure 4.15: Proposed optimum heat exchanger network

4.3 MegaMethanol

As explained in Chapter 3.3 it was important to see that MATLAB and UniSim would yield the same results for the BWR. The script for simulating the BWR in MATLAB, and comparing these values with UniSim is found in Appendix C and D. The results are seen in Figure 4.16 and 4.17.

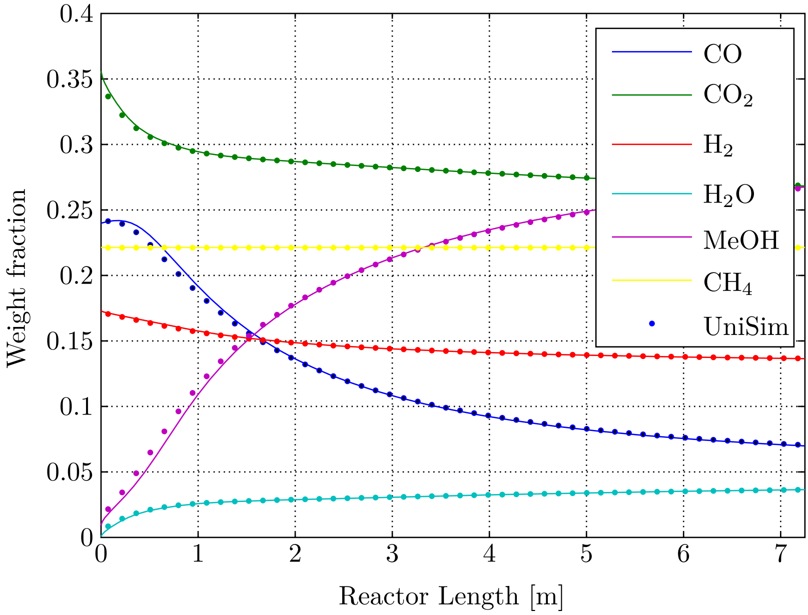

Figure 4.16: Weight fractions in the BWR from UniSim and MATLAB

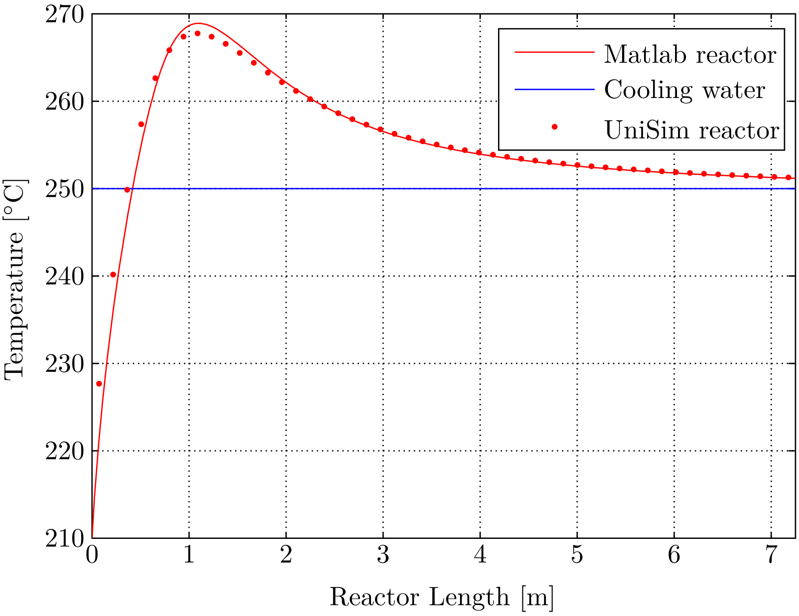

Figure 4.17: Temperatures in the BWR from UniSim and MATLAB

From Figure 4.16 and 4.17 it can be concluded that MATLAB and UniSim calculates approximately the same values.

Collocation was used to simulate the GCR. The MegaMethanol process was then simulated by combining the simulation of the recycle loop with the simulation of the GCR. The resulting script is found in Appendix E together with the UniSim flowsheet and databook. Results from this simulation is seen in Figure 4.18–4.21.

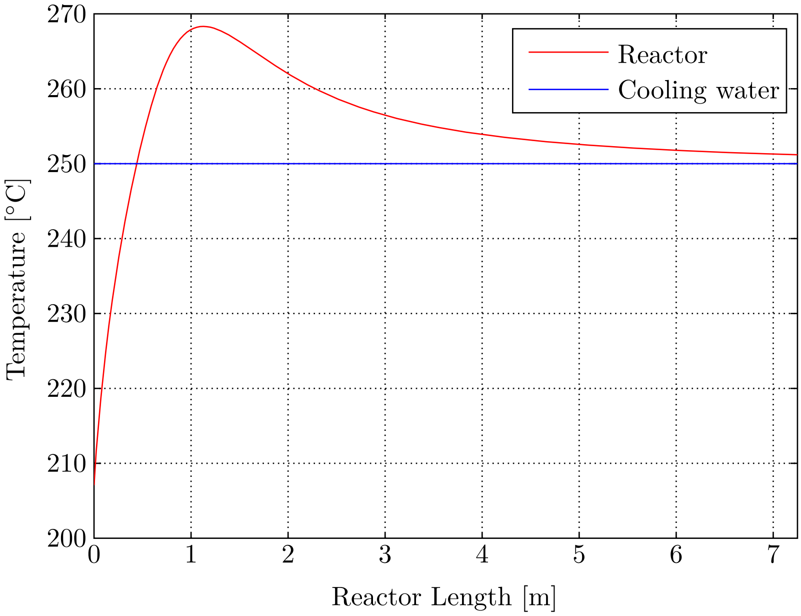

Figure 4.18: Temperature profile in the BWR

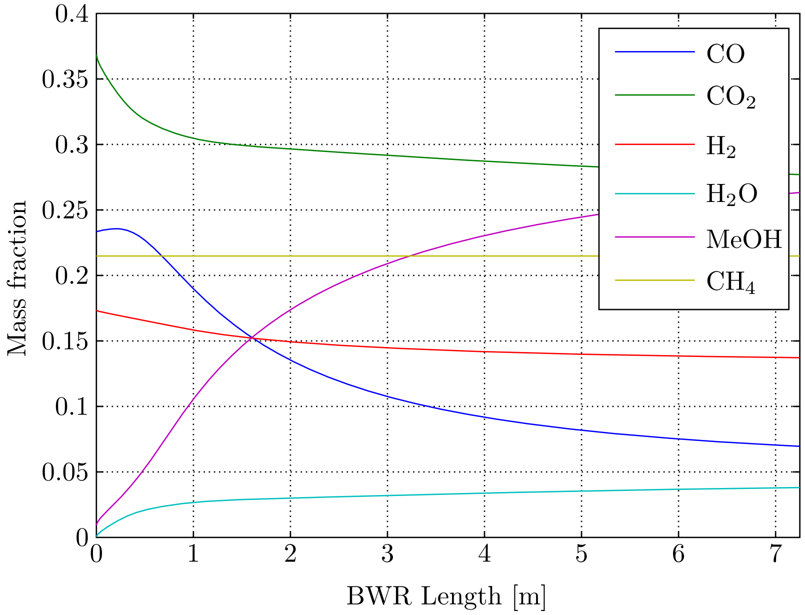

Figure 4.19: Weight fractions in the BWR

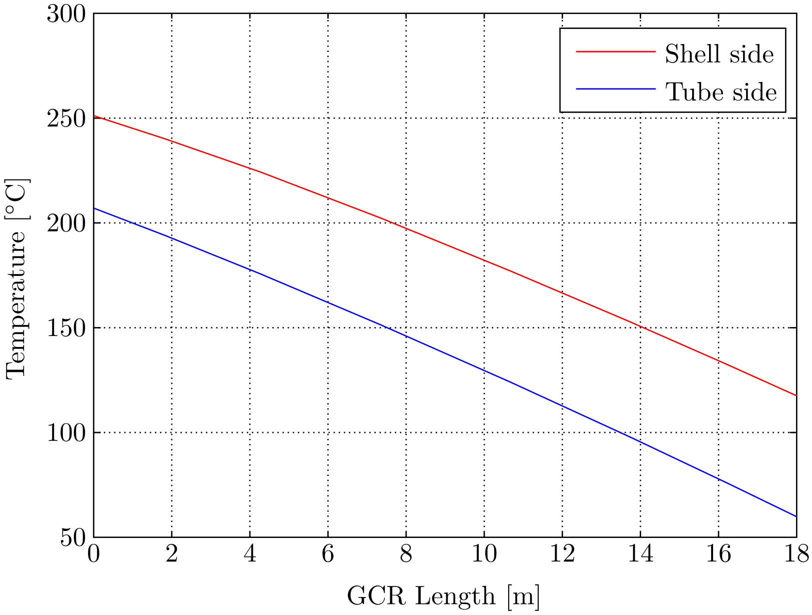

Figure 4.20: Temperature profile in the GCR

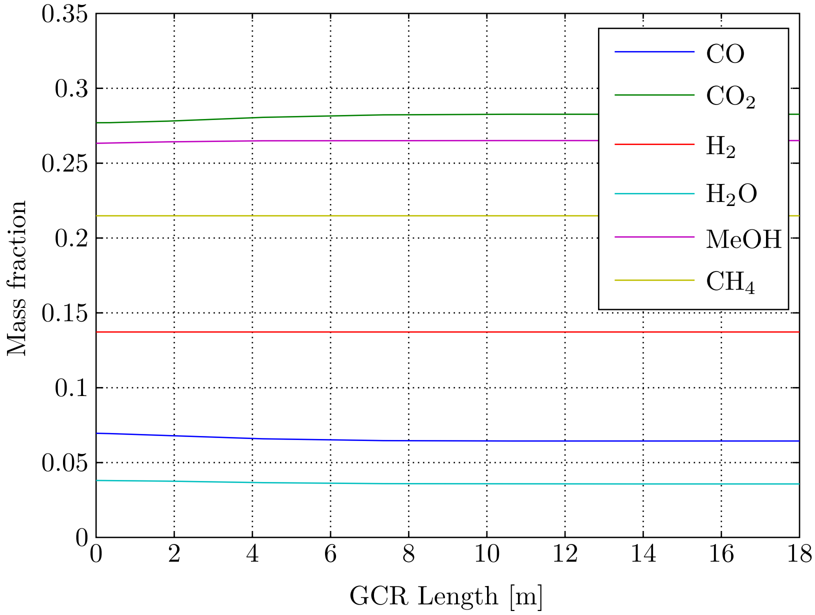

Figure 4.21: Weight fractions in the GCR

Figure 4.18 and 4.19 corresponds to Figure 4.17 and 4.16 meaning that there are little change in the BWR from the base case to the MegaMethanol process. The temperature profile in the GCR, shown in Figure 4.20, demonstrate that the shell side temperature has a steep decline from the start of the reactor. This indicates that little heat is produced from the reaction in the GCR. This is also seen as the small changes in weight fractions in Figure 4.21. When the shell side temperature in the GCR is below 250 °C the reaction kinetics decreases rapidly and limits the methanol production. This is demonstrated in Figure 4.22 where the cooling water for the BWR in the base case is varied, and the resulting methanol production is mapped. It becomes clear from this figure that the GCR temperatures are far from ideal for methanol production. From the simulation it is calculated that the GCR produces 0.69 tonne/h while the BWR produces 98.83 tonne/h. Compared to the base case, this is a total increase of 0.2 tonne/h. The small amount of extra methanol produced will not be enough to make the MegaMethanol process profitable.

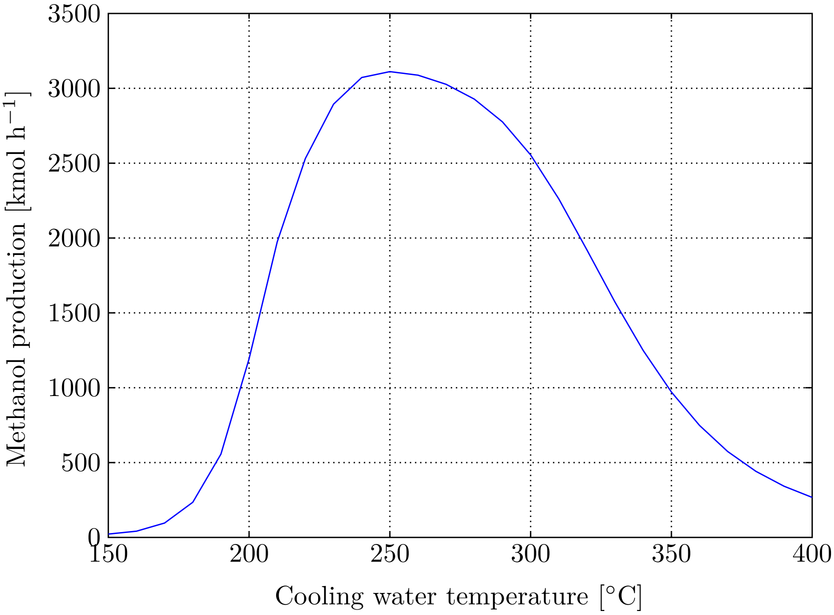

Figure 4.22: Methanol production as a function of cooling water temperature

Chapter 5

Conclusion

Simulations of the three different methanol reactor loop layouts was performed and it was concluded that:

- The base case simulation using kinetics from Vanden Bussche and Froment (1996) gave reasonable results compared to Tjeldbergodden methanol plant.
- An equal reactor length of 7.25 m produced the most methanol for the interstage methanol removal configuration.
- A case study of the cooling water temperatures for the two reactors in series showed that a temperature of 250°C in the first reactor and 255°C in the second reactor resulted in the largest methanol production.
- A recycle ratio of 2 seems to be a reasonable value for the interstage methanol removal configuration.
- The interstage methanol removal configuration produced 2.8 tonne/h (87 kmol/h) more methanol than the base case, resulting in a net present worth of over 47 million dollars over a 10 year horizon.
- It was proven that the addition of a GCR only increased the methanol production by 0.2 tonne/h. This will not be enough to make the MegaMethanol process profitable

List of symbols

a	Activity
A	Area
C_p^0 (gas)	Standard molar heat capacity at constant pressure
D	Diameter
LD_{50}	Lethal Dose 50%
M_w	Molecular weight
R	Recycle ratio
$\tilde{R}$	Mass reaction rate
r	Weight based reaction rate
r'	Volume based reaction rate
r_{Actual}	Actual (Observed) reaction rate
r_s	Reaction rate at surface conditions
S^0 (gas)	Standard entropy
SN	Stoichiometric number
t	Time
T	Temperature
T_c	Cooling water temperature
U	Overall heat transfer coefficient
v'	Superficial velocity
V	Volume
w	Weight fraction
W	Mass flow
ΔP	Pressure drop
$\Delta_{vap}H^0$	Molar enthalpy of vaporisation
$\Delta_f G^0$ (gas)	Standard Gibbs energy of formation
$\Delta_f H^0$ (gas)	Standard enthalpy of formation
ΔH_{rx}	Heat of reaction
ϵ	Void fraction
η	Internal efficiency factor
ψ	Sphericity

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Vanden Bussche, K. and G. Froment (1996). A steady-state kinetic model for methanol synthesis and the water gas shift reaction on a comercial Cu/ZnO/Al_2O_3 catalyst. *Journal of Catalysys 161*(0156), 1–10.

Appendix A

Interchanger pressure drop

To calculate the pressure drop on the tube side in the heat exchanger the following equation was used (Sinnott and Towler, 2009):

$$\Delta P_t = N_p \left[8 j_f \left(\frac{L}{d_i} \right) \left(\frac{\mu}{\mu_w} \right)^{-m} + 2.5 \right] \frac{\rho u_t^2}{2} \tag{A.1}$$

For the shell side:

$$\Delta P_s = 8 j_f \left(\frac{D_s}{d_e} \right) \left(\frac{L}{l_b} \right) \frac{\rho u_s^2}{2} \left(\frac{\mu}{\mu_w} \right)^{-0.14} \tag{A.2}$$

The following assumptions where made:

- 1.5 velocity head pressure drop for nozzles
- Square pitch
- 35% bafflecut
- neglected viscosity correction at wall
- 2.5 velocity heads per pass
- 2.5 m baffle spacing

Values produced from excel for the base case:

Table A.1: Tube side values

	Value	Unit
Number of tube side passes	1	
Number of tubes	5 412	
Tube length	18.00	m
Tube inner diameter	0.019	m
Fluid viscosity	$1.74 \cdot 10^{-5}$	Pa s
Fluid viscosity at wall	$1.74 \cdot 10^{-5}$	Pa s
jf	0.027	
m	0.14	
Average density	23.10	kg m^{-3}
Vol stream 4	22 110	m^3 h^{-1}
Vol stream 5	15 976	m^3 h^{-1}
Average vol flow	19 043	m^3 h^{-1}
Average vol flow	5.29	m^3 h^{-1}
Velocity	3.45	m s^{-1}
Re	87 048	
pressure drop	28 641	Pa
pressure drop	0.286	bar

Table A.2: Shell side values

	Value	Unit
Tube pitch	0.04	
Tube outside diameter	0.02	m
Shell inside diameter	2.50	m
Baffle spacing	2.25	m
Cross flow area	2.47	m^2
Mass flow	119.34	kg s^{-1}
Mass velocity	48.37	kg s^{-1} m^{-2}
Density	22.73	kg m^{-3}
Linear velocity	2.13	m s^{-1}
Hydraulic diameter	0.07	m
Viscosity	$1.41 \cdot 10^{-5}$	Pa s
Fluid viscosity at wall	$1.41 \cdot 10^{-5}$	
Re	248 846	
jf	0.25	
Pressure drop	28 281	Pa
Pressure drop	0.283	bar

For the interstage methanol removal the following values were obtained for HE-1:

Table A.3: Tube side values

	Value	Unit
Number of tube side passes	1	
Number of tubes	5 412	
Tube length	18.00	m
Tube inner diameter	0.019	m
Fluid viscosity	1.26E-05	Pa s
Fluid viscosity at wall	1.26E-05	Pa s
jf	0.032	
m	0.14	
Average density	19.92	kg m^{-3}
Vol stream 8	11666	m^3 h^{-1}
Vol stream 9	8194	m^3 h^{-1}
Average vol flow	9930	m^3 h^{-1}
Average vol flow	2.76	m^3 h^{-1}
Velocity	1.80	m s^{-1}
Re	53 861	
pressure drop	7 933	Pa
pressure drop	0.079	bar

Table A.4: Shell side values

	Value	Unit
Tube pitch	0.04	m
Tube outside diameter	0.02	m
Shell inside diameter	2.50	m
Baffle spacing	2.25	m^2
Cross flow area	2.47	kg s^{-1}
Mass flow	73.15	kg s^{-1} m^{-2}
Mass velocity	29.65	kg m^{-3}
Density	22.15	m s^{-1}
Linear velocity	1.34	m
Hydraulic diameter	0.07	Pa s
Viscosity	1.45E-05	
Fluid viscosity at wall	1.45E-05	
Re	149 316	
jf	0.27	Pa
Pressure drop	11 777	bar
Pressure drop	0.118	bar

A pressure drop of 0.2 bar was used in both heat exchangers, because it was concluded to simulate the worst case scenario.

Appendix B

Reaction Kinetics

In the basis environment in UniSim under the reaction tab, all the reactions of interest must be implemented. There are different ways of specifying these reactions, such as equilibrium reaction, kinetic reaction, conversion reaction or as in this case a heterogeneous catalytic reaction. Since there are many different ways of setting up the reaction rate for a heterogeneous catalytic reaction, the reaction rate expression has been generalized in UniSim. The general reaction rate expression is

$$\text{Reaction rate} = \frac{k \cdot f\left(Basis\right) - k' \cdot f'\left(Basis\right)}{\left(1 + K_1 \cdot f_1\left(Basis\right) + K_2 \cdot f_2\left(Basis\right) + ...\right)^n} \tag{B.1}$$

Where

$$\begin{aligned} k &= A \cdot \exp\left(-E/RT\right) \cdot T^{\beta} \\ k' &= A' \cdot \exp\left(-E'/RT\right) \cdot T^{\beta'} \\ K_1 &= A_1 \cdot \exp\left(-E_1/RT\right) \\ &\vdots \\ K_5 &= A_5 \cdot \exp\left(-E_5/RT\right) \end{aligned}$$

The functions $f(Basis)$, $f'(Basis)$, $f_1(Basis)$, $f_2(Basis)$, $\ldots$ are the product of the concentrations (fugacity, partial pressure, ...) to the power of the exponent given by the kinetic model.

The relevant reactions for methanol synthesis are:

$$\text{Reaction A} \qquad CO + 2\,H_2 \rightleftharpoons CH_3OH \tag{B.2}$$

$$\text{Reaction B} \qquad CO_2 + H_2 \rightleftharpoons CO + H_2O \tag{B.3}$$

$$\text{Reaction C} \qquad CO_2 + 3\,H_2 \rightleftharpoons CH_3OH + H_2O \tag{B.4}$$

In the article of Vanden Bussche and Froment (1996) the reaction rate for methanol production is derived from the hydrogenation of CO_2 (Reaction B.4) and the reverse water gas shift reaction (Reaction B.3). The reason for this is studies performed with labelled ^{14}C isotopes and Vanden Bussche and Froment (1996) used these results to eliminate CO as a carbon source. The developed intrinsic reaction rates are

$$\begin{aligned} r_C &= \frac{k_a p_{CO_2} p_{H_2} \left[1 - (1/K_1^*)\left(p_{H_2O} p_{CH_3OH} / p_{H_2}^3 p_{CO_2}\right)\right]}{\left(1 + k_c\left(p_{H_2O}/p_{H_2}\right) + \sqrt{k_d p_{H_2}} + k_e p_{H_2O}\right)^3} \\ r_B &= \frac{k_b p_{CO_2}\left[1 - K_3^*\left(p_{H_2O} p_{CO} / p_{CO_2} p_{H_2}\right)\right]}{\left(1 + k_c\left(p_{H_2O}/p_{H_2}\right) + \sqrt{k_d p_{H_2}} + k_e p_{H_2O}\right)} \end{aligned}$$

Since the reaction rates must be on the form of Equation B.1, these expressions are manipulated to

$$\begin{aligned} r_C &= \frac{k_a p_{CO_2} p_{H_2} - \frac{k_a}{K_1^*}\frac{p_{H_2O} p_{CH_3OH}}{p_{H_2}^2}}{\left(1 + k_c\left(p_{H_2O}/p_{H_2}\right) + \sqrt{k_d p_{H_2}} + k_e p_{H_2O}\right)^3} \\ r_B &= \frac{k_b p_{CO_2} - k_b K_3^* \frac{p_{H_2O} p_{CO}}{p_{H_2}}}{\left(1 + k_c\left(p_{H_2O}/p_{H_2}\right) + \sqrt{k_d p_{H_2}} + k_e p_{H_2O}\right)} \end{aligned}$$

Hydrogenation of Carbon Dioxide

The equilibrium constant for Reaction B.4 is found in Graaf et al. (1986) and is

$$\begin{aligned} \log\left(K_1^*\right) &= \frac{3066}{T} - 10.592 \\ \ln\left(K_1^*\right) &= \frac{3066 \cdot \ln(10)}{T} - 10.592 \cdot \ln(10) = \frac{7060}{T} - 24.39 \\ K_1^* &= 2.56 \cdot 10^{-11} exp\left(\frac{58695}{RT}\right) \end{aligned}$$

$$\frac{k_a}{K_1^*} = \frac{1.07 \exp\left(\frac{36696}{RT}\right)}{2.56 \cdot 10^{-11} \exp\left(\frac{58695}{RT}\right)} = 4.18 \cdot 10^{10} \exp\left(\frac{-21999}{RT}\right)$$

$$r_C = \frac{1.07 \exp\left(\frac{36696}{RT}\right) p_{CO_2} p_{H_2} - 4.18 \cdot 10^{10} \exp\left(\frac{-21999}{RT}\right) p_{H_2O} p_{CH_3OH} p_{H_2}^{-2}}{\left(1 + 3453.38 p_{H_2O} p_{H_2}^{-1} + 0.499 \exp\left(\frac{17197}{RT}\right) p_{H_2}^{-0.5} + 6.62 \cdot 10^{-11} \exp\left(\frac{124119}{RT}\right) p_{H_2O}\right)^3}$$

UniSim allows different units for the reaction rate, but they are all on volume basis. The unit kmol$\cdot$ s$^{-1}\cdot$ m^{-3} was chosen, and it was discovered that m^{-3} means void volume of the reactor. The reaction rates from Vanden Bussche and Froment (1996) have the units mol$\cdot$ s$^{-1}\cdot$ kg^{-1} and therefore must be multiplied with the solid density of the catalyst, multiplied by the catalyst volume over the void volume and divided by 1000 (Since UniSim uses kmol instead of mol).

$$
\begin{aligned}
r_C &[=] \frac{mol}{kgcat \cdot s} \\
r_C' &= r_C \cdot \rho_c \cdot \frac{1-\epsilon}{\epsilon} \cdot \frac{1\text{kmol}}{1000\text{mol}} \\
r_C' &[=] \frac{kmol}{m_v^3 \cdot s}
\end{aligned}
$$

Where $\rho_C = 1950$ is the density of the catalyst, ϵ is the void fraction and m_v^3 is the void volume.

$$
r_C = \frac{3.13 \exp\left(\frac{36696}{RT}\right) p_{CO_2} p_{H_2} - 1.22 \cdot 10^{11} \exp\left(\frac{-21999}{RT}\right) p_{H_2O} p_{CH_3OH} p_{H_2}^{-2}}{\left(1 + 3453.38 p_{H_2O} p_{H_2}^{-1} + 0.499 \exp\left(\frac{17197}{RT}\right) p_{H_2}^{0.5} + 6.62 \cdot 10^{-11} \exp\left(\frac{124119}{RT}\right) p_{H_2O}\right)^3}
$$

Reverse Water Gas Shift Reaction

The equilibrium constant for the reverse of Reaction B.3 is found in Graaf et al. (1986) and is

$$
\begin{aligned}
\log\left(\frac{1}{K_3^*}\right) &= \frac{-2073}{T} + 2.029 \\
\ln\left(K_3^*\right) &= \frac{2073 \cdot \ln(10)}{T} - 2.029 \ln(10) = \frac{4773}{T} - 4.672 \\
K_3^* &= 9.35 \cdot 10^{-3} exp\left(\frac{39685}{RT}\right)
\end{aligned}
$$

$$
k_b K_3^* = 1.22 \cdot 10^{10} \exp\left(\frac{-94765}{RT}\right) \cdot 9.35 \cdot 10^{-3} \exp\left(\frac{39685}{RT}\right) = 1.14 \cdot 10^{8} \exp\left(\frac{-55080}{RT}\right)
$$

$$
r_B = \frac{1.22 \cdot 10^{10} \exp\left(\frac{-94765}{RT}\right) p_{CO_2} - 1.14 \cdot 10^{8} \exp\left(\frac{-55080}{RT}\right) p_{H_2O} p_{CO} p_{H_2}^{-1}}{1 + 3453.38 p_{H_2O} p_{H_2}^{-1} + 0.499 \exp\left(\frac{17197}{RT}\right) p_{H_2}^{0.5} + 6.62 \cdot 10^{-11} \exp\left(\frac{124119}{RT}\right) p_{H_2O}}
$$

$$
\begin{aligned}
r_B &[=] \frac{mol}{kgcat \cdot s} \\
r_B' &= \cdot \rho_c \cdot \frac{1-\epsilon}{\epsilon} \cdot \frac{1\text{kmol}}{1000\text{mol}} \\
r_B' &[=] \frac{kmol}{m_v^3 \cdot s}
\end{aligned}
$$

Where ρ_C is the density of the catalyst, ϵ is the void fraction and m_v^3 is the reactor volume.

$$
r_B' = \frac{3.57 \cdot 10^{10} \exp\left(\frac{-94765}{RT}\right) p_{CO_2} - 3.34 \cdot 10^{8} \exp\left(\frac{-55080}{RT}\right) p_{H_2O} p_{CO} p_{H_2}^{-1}}{1 + 3453.38 p_{H_2O} p_{H_2}^{-1} + 0.499 \exp\left(\frac{17197}{RT}\right) p_{H_2}^{0.5} + 6.62 \cdot 10^{-11} \exp\left(\frac{124119}{RT}\right) p_{H_2O}}
$$

UniSim Input Values

The input values for the nominator is multiplied by the value of $a\eta = 0.7$ in Reaction B.3 and Reaction B.4. The input values then becomes

Table B.1: Nominator values for reaction B.3

Constant	Value	Components	Forward Order	Reverse Order
A	2.19	CO	0	0
E	-36696	CO_2	1	0
A'	$8.56 \cdot 10^{10}$	H_2	1	-2
E'	21999	H_2O	0	1
β , β'	0	CH_3OH	0	1

Table B.2: Nominator values for reaction B.4

Constant	Value	Components	Forward Order	Reverse Order
A	$2.50 \cdot 10^{10}$	CO	0	1
E	94765	CO_2	1	0
A'	$2.34 \cdot 10^{8}$	H_2	0	-1
E'	55080	H_2O	0	1
β , β'	0	CH_3OH	0	0

The denominator values are

Table B.3: Denominator values

i	A_i	E_i $[Jmol^{-1}]$	CO	CO_2	H_2	H_2O	CH_3OH
1	3453.38	0	0	0	-1	1	0
2	0.499	-17197	0	0	0.5	0	0
3	$6.62 \cdot 10^{-11}$	-124119	0	0	0	1	0

The denominator exponent is 3 for CO_2 hydrogenation and 1 for the RWGS reaction.

Appendix C

MATLAB and UniSim comparison script

```
clear all
clc

global a

Pfeed   = 80;                                %[bar]
Tfeed   = 210.0134;                          %[C]
myfeed  = 1.566e−05;                         %[Pa∗s]
a.Wcomp = [25.89,38.41,18.67,0.0683,1.0037,23.89];
a.Wcomp = a.Wcomp(1:6);
%          CO     CO2    H2     H2O    MeOH   CH4
a.M    = [28.010 44.010 2.016  18.016 32.042 16.042];%[kg/kmol]
a.n    = 6;                                  % # components
a.cpm = [1.073 1.025 14.51 1.975 1.9 3];     % cp [kJ/kg−K]
a.Wflow = sum(a.Wcomp);                      % feed flow [kg/s]
a.w0    = a.Wcomp'/a.Wflow;                  % mass frac at inlet [−]
a.T0BWR = Tfeed;                             % temp at inlet [C]
a.P0    = Pfeed;                             % pres at inlet [bara]
a.Tw0   = 250;                               % cooling water T [C]
x0      = [a.w0; a.T0BWR; a.P0; a.Tw0];      % initial conditions
a.dHr   = [−49.6 41.0]∗1e3;                  % Heat of reac [kJ/kmol]
a.d     = 40.5e−3;                           % inner diam [m]
a.S     = pi∗(a.d/2.0)^2;                    % cross section [m2]
a.Vtube = a.S∗7.25;                          % tube volume [m3]
a.Ntubes= 5515∗2;                            % Number of tubes [−]
a.Vreact= a.Vtube∗a.Ntubes;                  % Reactor volume [m3]
a.ph    = 4e−3;                              % pellet height [m]
a.dp    = 6e−3;                              % pellet diam [m]
a.eps   = 0.40;                              % void fraction [−]
a.my    = myfeed;                            % gas viscosity [Pa∗s]
a.U     = 1000;                              % over heat trans [W/m2∗K]
a.rhoC  = 1950;                              % cat solid dens [kg/m3]
a.rhoB  = a.rhoC∗(1−a.eps);                  % bulk solid dens [kg/m3]
a.Vp    = pi∗(a.dp/2)^2∗a.ph;                % Pellet vol [m3]
```

```
a.Ap    = (2*pi*(a.dp/2)^2)+(2*pi*(a.dp/2)*a.ph);% surf area [m2]
a.spheri= (pi^(1/3)*(6*a.Vp)^(2/3))/(a.Ap); % sphericity [-]
a.Fc    = 1e9;                            %Coolant mol flow [kmol/s]
a.Cpc   = 87.76;                          % Coolant Cp [kJ/kmol*C]

opt=odeset('AbsTol',1e-5,'RelTol',1.e-5);
[V X]=ode45(@pfr,[0 a.Vreact],x0,opt);

w = X(:,1:a.n);
y = mass2mol(w,a.M');
L=V/(a.S*a.Ntubes);
P=X(:,a.n+2);
T=X(:,(a.n+1));
Tc=round(X(:,a.n+3));

load UniSim                               % Values from the BWR in ...
    UniSim

LU=UniSim(:,1);
wUniSim=UniSim(:,2:7);
TUniSim=UniSim(:,8);

% Plot weight fractions from UniSim and MATLAB
figure(1)
plot(L,w(:,1),L,w(:,2),L,w(:,3),L,w(:,4),L,w(:,5),L,w(:,6),'y')
hold on
plot(LU,wUniSim(:,1),'.',LU,wUniSim(:,2),'.',LU,wUniSim(:,3),'.',...
    LU,wUniSim(:,4),'.',LU,wUniSim(:,5),'.',LU,wUniSim(:,6),...
    'y.','MarkerSize',15)
hold off
xlabel('Reactor Length [m]')
ylabel('Weight fraction')
legend('CO','CO_2','H_2','H_2O','MeOH','CH_4','UniSim')
grid on
xlim([0 7.25])

% Save the figure as pgf
matfig2pgf...
('C:\...\Grafer\matlabwf')

% Plot the temperature profile from UniSim and MATLAB
figure(2)
plot(L,T,'r',L,Tc,'b',LU,TUniSim,'.r','MarkerSize',15)
xlabel('Reactor Length [m]')
ylabel('Temperature [^{\circ}C]')
legend('Matlab reactor','Cooling water','UniSim reactor')
grid on
xlim([0 7.25])

% Save the figure as pgf
matfig2pgf...
('C:\...\Grafer\matlabT')
```

Appendix D

MATLAB PFR

```
function [f]=pfr(V,x)
%―――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――
% name          : Calculating the derivatives for the PFR reactor.
% author        : Kristian Bøhn
% date          : 08.03.2011
% last time rev : 25.05.2011
% input:
% V             : Reactor volume             [m3]
% x(1:n)        : Gas composition            [mass frac]
% x(n+1)        : Temperature                [C]
% x(n+2)        : Pressure                   [bar]
% x(n+3)        : Cooling water temp         [C]
% a             : Struct with parameters given in the main program
% output:
% dwdV          : Weight fraction change per reactor volume     [1/m3]
% dTdV          : Temperature change per reactor volume        [K/m3]
% dPdV          : Pressure change per reactor volume           [bar/m3]
% dTcdV         : Cooling medium temp change per reac volume  [K/m3]
%―――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――――
global a

n  = a.n;
w  = x(1:n);
T  = x(n+1);
%P  = x(n+2);
Tc = x(n+3);

% Call function to calculate pressure drop
[dPdL]=pressdrop(x);

% Call function giving the reaction rates
[R r]=reactionrates(x);        % R reaction rates [kg/m3*s]

dwdV  = R/a.Wflow;
dTdV  = (−a.dHr*r − a.U/1000 * 4/a.d * (T−Tc))/(a.Wflow*a.cpm*w);
dPdV  = (dPdL/(a.S*a.Ntubes));
dTcdV = (a.U/1000*4/a.d*(Tc−T))/(a.Fc*a.Cpc);
```

```
f     = [dwdV;
        dTdV
        dPdV
        dTcdV];
end


function dPdL = pressdrop(x)
%-----------------------------------------------------------------------
% name           : Calculating turbulent pressure drop using Erguns Eq.
% author         : Kristian Bøhn
% date           : 21.03.2011
% last time rev  : 25.05.2011
% input:
%   x(1:n)       : Weight fractions
%   x(n+1)       : Temperature           [C]
%   x(n+2)       : Pressure              [bar]
%   a.M(1:6)     : Molecular weight      [kg/kmol]
%   T0           : Start temperature     [C]
%   P0           : Start pressure        [bar]
%   w0           : Start mass fractions  [-]
% output:
%   dPdL         : Pressure drop per length
%-----------------------------------------------------------------------
global a

n  = a.n;
w  = x(1:n);
T  = x(n+1);
P  = x(n+2);

R=8.314;                                                % [J/(K*mol)]
T0 = a.T0BWR;
Wflow   = a.Wflow;
Mw      = inv(sum(w./a.M'));
F0      = Wflow*sum(a.w0./a.M');
F       = Wflow./Mw;
rhog    = (P*1e5.*(Mw))./(R.*(T+273.15));               % [g/m3]
rhog    = rhog/1000;                                    % [kg/m3]
VFlow   = Wflow./rhog;                                  % [m3/s]

% Calculate superficial velocity
v     = (VFlow/(a.S*a.Ntubes))*(F/F0)*(a.P0./P)*((T+273)/(T0+273));

% Turbulent pressure drop [bar]
dPturb=((1.75*rhog.*(v^2)*(1-a.eps))/(a.dp*a.spheri*(a.eps^3)))/1e5;

dPdL    = -(dPturb);                                    %[bar]
end


function [R r]=reactionrates(x)
%-----------------------------------------------------------------------
% name           : Vanden Bussche and Froment Reaction Kinetics
% author         : Kristian Bøhn
% date           : 18.03.2011
```

```
% last time rev : 25.05.2011
% input:
%   x(1)         : Mass fraction of CO
%   x(2)         : Mass fraction of CO2
%   x(3)         : Mass fraction of H2
%   x(4)         : Mass fraction of H2O
%   x(5)         : Mass fraction of CH3OH
%   x(6)         : Mass fraction of CH4
%   x(7)         : Temperature       [C]
%   x(8)         : Pressure          [bar]
%   a.M(1:6)     : Molecular weight  [kg/kmol]
% output:
%   r(1)     : rate of reaction 1 [kmol/(m3*s)] CO2 + 3H2 = CH3OH + H2O
%   r(2)     : rate of reaction 2 [kmol/(m3*s)] CO2 + H2 = CO + H2O
%   R(i)     : component reaction rates [kg/(m3*s)] (i=1..6)
%----------------------------------------------------------------------
global a

sumMol = sum(x(1:a.n)./a.M(1:a.n)');
xCO    = x(1)/a.M(1)/sumMol;
xCO2   = x(2)/a.M(2)/sumMol;
xH2    = x(3)/a.M(3)/sumMol;
xH2O   = x(4)/a.M(4)/sumMol;
xMeOH  = x(5)/a.M(5)/sumMol;

T      = x(a.n+1)+273;                      %[K]
Pres   = x(a.n+2);                          %[bar]
R      = 8.314;                             %[J/(K*mol)]
pCO    = Pres*xCO;
pCO2   = Pres*xCO2;
pH2    = Pres*xH2;
pH2O   = Pres*xH2O;
pMeOH  = Pres*xMeOH;

% Rate constants
K1=1.07*exp(36696/(R*T));
K2=4.18e10*exp(-21999/(R*T));
K3=1.22e10*exp(-94765/(R*T));
K4=1.14e8*exp(-55080/(R*T));

% Compute the denominator
denom1=1+(3453.38*pH2O*pH2^(-1));
denom2=(0.499*exp(17197/(R*T))*pH2^(0.5));
denom3=(6.62e-11*exp(124119/(R*T))*pH2O);
denom=denom1+denom2+denom3;

% Compute the reaction rates [mol/(kg cat*s)]
r=zeros(2,1);
r(1)    = (K1*pCO2*pH2 - K2*pH2O*pMeOH*pH2^(-2))/(denom^3);
r(2)    = (K3*pCO2 - K4*pH2O*pCO*pH2^(-1))/denom;

% Internal efficiency factor * activity = ua = 0.7;
r=r*0.7*(a.rhoB/1000);                    % now [r] is kmol/(m3*s)

% component rates
g  = [r(2);                    % CO   1
      -r(1)-r(2);              % CO2  2
```

```
      -3*r(1)-r(2);           % H2   3
      r(1)+r(2);              % H2O  4
      r(1);                   % MeOH 5
      0];                     % CH4  6

R       = g.*a.M';            % [kg/m3*s] where m3 is for empty reactor
end
```

Appendix E

Mega Methanol

If the commando for the material stream property is unknown, the fieldnames commando is very practical. E.g. writing fieldnames(g.Item('2')) in MATLAB yields every possible command for stream 2.

```
clear all
clc

global a b g

h                = actxserver('UnisimDesign.Application');
hyCase           = h.Activedocument;
sol              = hyCase.Solver;
f                = hyCase.Flowsheet;
g                = f.MaterialStreams;
sol.CanSolve     = 1;

%%%%%%%%%%%%  Component properties  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%         CO     CO2    H2     H2O    MeOH   CH4
a.M   = [28.010 44.010 2.016  18.016 32.042 16.042]; % [kg/kmol]
a.cpm = [1.064 1.014 14.51 1.954 1.9 2.889];%mass Cp at 500 K [kJ/kgK]
a.n     = 6;                                % number of components
a.dHr   = [−49.6 41.0]*1e3;                 % heat of reac [kJ/kmol]
a.my    = g.Item('2').ViscosityValue*0.001; % gas viscosity [Pa*s]

%%%%%%%%%%%%  Water cooled reactor specifications  %%%%%%%%%%%%%%%%%%
a.d     = 40.5e−3;                          % inner diam [m]
a.S     = pi*(a.d/2.0)^2;                   % cross section [m2]
a.Vtube = a.S*7.25;                         % tube volume [m3]
a.Ntubes= 5515*2;                           % number of tubes [−]
a.Vreact= a.Vtube*a.Ntubes;                 % reactor volume [m3]
a.ph    = 4e−3;                             % pellet height [m]
a.dp    = 6e−3;                             % pellet diam [m]
a.eps   = 0.40;                             % void fraction [−]
a.U     = 1000;                             % over heat trans [W/m2*K]
a.rhoB  = 1950*(1−a.eps);                   % bulk solid dens [kg/m3]
a.Vp    = pi*(a.dp/2)^2*a.ph;               % pellet vol [m3]
a.Ap    = (2*pi*(a.dp/2)^2)+(2*pi*(a.dp/2)*a.ph); % surf area [m2]
```

```
a.spheri= (pi^(1/3)*(6*a.Vp)^(2/3))/(a.Ap); % sphericity [-]
a.Tw0   = 250;                              % cooling water T [C]
a.Fc    = 1e9;                              % cool. mol flow [kmol/s]
a.Cpc   = 87.76;                            % coolant Cp [kJ/kmol*C]

%%%%%%%%%%%%  Gas cooled reactor specifications %%%%%%%%%%%%%%%%%%%%%%
b.z       = 18;                             % length of reactor [m]
b.Ntubes  = 5412;                           % number of tubes [-]
b.d       = 19e-3;                          % tube inner diameter[m]
b.Vc      = b.Ntubes*pi*(b.d/2)^2*b.z;      % tube volume [m3]
b.do      = 29e-3;                          % tube outer diameter [m]
b.Vco     = b.Ntubes*pi*(b.do/2)^2*b.z;     % tube outer volume [m3]
b.Dshell  = 2.7-0.2;                        % shell diameter [m]
b.Vtot    = pi*(b.Dshell/2)^2*b.z;          % total shell vol [m3]
b.Vr      = b.Vtot-b.Vco;                   % reactor volume [m3]
% Over heat trans [W/m2*K] from p.821 in Sinnott 5th ed.
b.U       = 200;                            % over heat trans [W/m2*K]

%%%%%%%%%%%%  Collocation  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%          [r, A, B, q] = colloc( n [,'left'] [,'right'])
% inputs:
%          n - number of interior node points
%          'left'  - include left boundary
%          'right' - include right bounary also
% outputs:
%           r - vector of roots
%           A - Matrix of first derivative weights
%           B - Matrix of second derivative weights
%           q - Quadrature weights.

n=8;
[xg,A,¬,¬]=colloc(n,1,1);

load tipp                  % Previously saved initial conditions

opt=optimset('Display','iter','TolFun',1e-5,'TolX',...
    1e-5 ,'MaxFunEvals',100000,'MaxIter ',20);

[x fval]=fsolve(@(x) residmega(x,A,n),tipp,opt);

%%%%%%%%%%%%  Results GCR  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
x=sqrt(x.^2);

L         = xg*b.z;                    % [m]
Tgh       = x(((n+2)*6)+1:(n+2)*7);    % [C]
Tgc       = x(((n+2)*7)+1:(n+2)*8);    % [C]
wh        = x(1:(n+2)*6);              % [-]
whCO      = wh(1:n+2);
whCO2     = wh((n+2)+1:(n+2)*2);
whH2      = wh(((n+2)*2)+1:(n+2)*3);
whH2O     = wh(((n+2)*3)+1:(n+2)*4);
whMeOH    = wh(((n+2)*4)+1:(n+2)*5);
whCH4     = wh(((n+2)*5)+1:(n+2)*6);

figure(1)
plot(L,Tgh,'r',L,Tgc,'b')
legend('Shell side','Tube side')
```

```
xlabel('GCR Length [m]')
ylabel('Temperature [^{\circ}C]')
grid on
xlim([0 18])
matfig2pgf('C:\...\Grafer\GCRtemp')

figure(2)
plot(L,whCO,L,whCO2,L,whH2,L,whH2O,L,whMeOH,L,whCH4)
legend('CO','CO_2','H_2','H_2O','MeOH','CH_4')
xlabel('GCR Length [m]')
ylabel('Mass fraction')
grid on
xlim([0 18])
matfig2pgf('C:\...\Grafer\GCRwf')

%%%%%%%%%%%%  Results BWR  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
LBWR   = a.V/(a.S*a.Ntubes);                     % [m]
w   = a.X(:,1:a.n);                              % [-]
P   = a.X(:,a.n+2);                              % [bar]
T   = a.X(:,a.n+1);                              % [C]
Tc  = a.X(:,a.n+3);                              % [C]

figure(3)
plot(LBWR,w)
xlabel('Reactor Length [m]')
ylabel('Mass fraction')
legend('CO','CO_2','H_2','H_2O','MeOH','CH_4')
grid on
xlim([0 7.25])

matfig2pgf('C:\...\Grafer\GCRBWRwf')

figure(4)
plot(LBWR,T,'r',LBWR,Tc,'b')
xlabel('Reactor Length [m]')
ylabel('Temperature [^{\circ}C]')
legend('Reactor','Cooling water')
grid on
xlim([0 7.25])

matfig2pgf('C:\...\Grafer\GCRBWRtemp')

%%%%%%%%%%%%  Methanol yield  %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
Wcomp   = x( ((n+2)*8)+1:((n+2)*8)+6);
a.Wflow = sum( Wcomp );
w0      = Wcomp./a.Wflow;
MeOHBWR = ((a.X(end,5)*a.Wflow) - (w0(5)*a.Wflow))*3.600;
MeOHGCR = (wh((n+2)*5)*a.Wflow - (a.X(end,5)*a.Wflow) )*3.600;



function res=residmega(x,A,n)
global a b g

% None of the values can be negative
x       = sqrt(x.^2);

wh      = x(1:(n+2)*6);                % [-]
```

```
Tgh     = x(((n+2)*6)+1:(n+2)*7);      % [C]
Tgc     = x(((n+2)*7)+1:(n+2)*8);      % [C]
Wcomp   = x( ((n+2)*8)+1:((n+2)*8)+6); % [kg/s]
a.Wflow = sum( Wcomp );
a.w0      = Wcomp./a.Wflow;
a.P0      = x(((n+2)*8)+7);
T0      = x(((n+2)*8)+8);
res=ones(length(x),1);


a.T0BWR   = Tgc(1);
x0      = [a.w0; a.T0BWR; a.P0; a.Tw0];% initial conditions for the BWR
opt=odeset('AbsTol',1e-6,'RelTol',1.e-3);
[V X]=ode45(@pfr,[0 a.Vreact],x0,opt);
a.V=V;
a.X=X;

Ph      = zeros(n+2,1)+X(end,8); %[bar]

res(1:(n+2):(n+2)*6)  = ...
    wh(1:(n+2):(n+2)*6) - X(end,1:6)';% left comp flow boundary cond
res(((n+2)*6)+1)  = Tgh(1) - X(end,7);% left temperature boundary cond

% n internal collocation points
for i = 2:n+2
    % reaction rates at each internal collocation point
     [R r]=reactionrates([wh(i:(n+2):(n+2)*6);Tgh(i);Ph(i)]);
    for k = 1:6
        % weight fraction at each internal collocation point
        res((n+2)*(k-1)+i) = ...
            A(i,:)*wh((n+2)*(k-1)+1:(n+2)*k)-R(k)*(b.Vr/a.Wflow);
    end
    % shell side temperature at each internal collocation point
    res(((n+2)*6)+(i):(n+2)*7) = A(i,:)*Tgh + ...
        (a.dHr*r*1000+ b.U*(4/b.d)*(Tgh(i)-Tgc(i)))*...
        (b.Vr/(a.Wflow*1000*a.cpm*(wh(i:(n+2):(n+2)*6))));
end

for i = 1:n+1
    % Tube side temperature at each internal collocation point
    res(((n+2)*7)+i:(n+2)*8) = A(i,:)*Tgc + ...
       (b.U*(4/b.d)*(Tgh(i)-Tgc(i)))*(b.Vc/(a.Wflow*1000*a.cpm*a.w0));
end

res((n+2)*8) = Tgc(n+2)-T0;% temperature at right boundary cond (Tube)

Whout=wh(n+2:n+2:(n+2)*6)*a.Wflow;
a.Whout=Whout;

% return values to UniSim
g.Item('5').PressureValue      = Ph(end)*100; % [kPa]
g.Item('5').TemperatureValue   = Tgh(end);     % [C]
g.Item('CO').MassFlowValue     = Whout(1);
g.Item('CO2').MassFlowValue    = Whout(2);
g.Item('H2').MassFlowValue     = Whout(3);
g.Item('H2O').MassFlowValue    = Whout(4);
g.Item('MeOH').MassFlowValue   = Whout(5);
```

```
g.Item('CH4').MassFlowValue     = Whout(6);

% get values from UniSim after recycle
Wci     = g.Item('2').ComponentMassFlowValue;
Pci     = g.Item('2').PressureValue/100;
Tci     = g.Item('2').TemperatureValue;

% calculate recycle residual
res( ((n+2)*8)+1:((n+2)*8)+8)=...
    [Wci Pci Tci]'-x(((n+2)*8)+1:((n+2)*8)+8);
end
```

The MegaMethanol simulation in UniSim is shown in Figure E, with the corresponding woorkbook below.

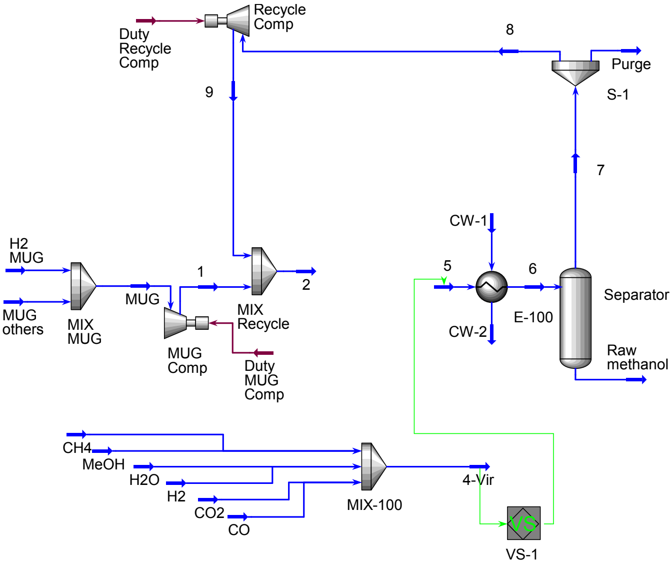


Figure E.1: UniSim simulation

Company Name Not Available
Calgary, Alberta
CANADA

Case Name:	C:\Users\...\UniSim\MegaMethanol Matlab.usc
Unit Set:	SI
Date/Time:	Monday Jun 6 2011, 11:21:28

Workbook: Case (Main)

Streams

Fluid Pkg: All

Name		MUG others	1	2	6	Raw methanol
Vapour Fraction		0.9987	1.0000	1.0000	0.8976	0.0000
Temperature	(C)	25.00 *	146.8	59.82	30.00 *	30.00
Pressure	(kPa)	3000 *	8000 *	8000	7903	7903
Molar Flow	(kgmole/h)	3498 *	1.132e+004	4.529e+004	3.908e+004	4001
Mass Flow	(kg/h)	1.106e+005	1.264e+005	3.890e+005	3.890e+005	1.178e+005
Std Ideal Liq Vol Flow	(m3/h)	142.8	368.6	1537	1352	145.3
Heat Flow	(kJ/h)	-6.472e+008	-6.049e+008	-2.016e+009	-2.469e+009	-1.010e+009
Molar Enthalpy	(kJ/kgmole)	-1.850e+005	-5.342e+004	-4.451e+004	-6.317e+004	-2.525e+005
Comp Mass Frac (CO)		0.6019 *	0.5268	0.2334	0.0644	0.0002
Comp Mass Frac (CO2)		0.3704 *	0.3242	0.3685	0.2827	0.0362
Comp Mass Frac (Hydrogen)		0.0000 *	0.1248	0.1734	0.1373	0.0003
Comp Mass Frac (H2O)		0.0016 *	0.0014	0.0006	0.0357	0.1174
Comp Mass Frac (Methanol)		0.0000 *	0.0000	0.0093	0.2651	0.8438
Comp Mass Frac (Methane)		0.0261 *	0.0228	0.2148	0.2148	0.0021
Name		7	Purge	9	8	5
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	0.9673
Temperature	(C)	30.00	30.00	31.64	30.00	117.5 *
Pressure	(kPa)	7903	7903	8020 *	7903	7923 *
Molar Flow	(kgmole/h)	3.508e+004	1110	3.397e+004	3.397e+004 *	3.908e+004
Mass Flow	(kg/h)	2.712e+005	8585	2.626e+005	2.626e+005	3.890e+005
Std Ideal Liq Vol Flow	(m3/h)	1206	38.18	1168	1168	1352
Heat Flow	(kJ/h)	-1.459e+009	-4.618e+007	-1.411e+009	-1.413e+009	-2.248e+009
Molar Enthalpy	(kJ/kgmole)	-4.158e+004	-4.158e+004	-4.153e+004	-4.158e+004	-5.751e+004
Comp Mass Frac (CO)		0.0923	0.0923	0.0923	0.0923	0.0644
Comp Mass Frac (CO2)		0.3898	0.3898	0.3898	0.3898	0.2827
Comp Mass Frac (Hydrogen)		0.1967	0.1967	0.1967	0.1967	0.1373
Comp Mass Frac (H2O)		0.0002	0.0002	0.0002	0.0002	0.0357
Comp Mass Frac (Methanol)		0.0137	0.0137	0.0137	0.0137	0.2651
Comp Mass Frac (Methane)		0.3072	0.3072	0.3072	0.3072	0.2148
Name		H2 MUG	MUG	CW-1	CW-2	MeOH
Vapour Fraction		1.0000	1.0000	0.0000	0.0000	1.0000
Temperature	(C)	25.00 *	22.20	15.00 *	50.00 *	250.0 *
Pressure	(kPa)	3000 *	3000	100.0 *	80.00	8000 *
Molar Flow	(kgmole/h)	7825 *	1.132e+004	8.136e+004	8.136e+004	3219
Mass Flow	(kg/h)	1.578e+004	1.264e+005	1.466e+006	1.466e+006	1.031e+005 *
Std Ideal Liq Vol Flow	(m3/h)	225.8	368.6	1469	1469	129.6
Heat Flow	(kJ/h)	-1.164e+004	-6.472e+008	-2.335e+010	-2.313e+010	-6.445e+008
Molar Enthalpy	(kJ/kgmole)	-1.488	-5.716e+004	-2.870e+005	-2.843e+005	-2.002e+005
Comp Mass Frac (CO)		0.0000 *	0.5268	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (CO2)		0.0000 *	0.3242	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (Hydrogen)		1.0000 *	0.1248	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (H2O)		0.0000 *	0.0014	1.0000 *	1.0000	0.0000 *
Comp Mass Frac (Methanol)		0.0000 *	0.0000	0.0000 *	0.0000	1.0000 *
Comp Mass Frac (Methane)		0.0000 *	0.0228	0.0000 *	0.0000	0.0000 *

Printed by: Kristian * Specified by user.

Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

Name		CH4	H2	CO	CO2	H2O
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	0.0000
Temperature	(C)	250.0 *	250.0 *	250.0 *	250.0 *	250.0 *
Pressure	(kPa)	8000 *	8000 *	8000 *	8000 *	8000 *
Molar Flow	(kgmole/h)	5210	2.649e+004	894.3	2499	771.7
Mass Flow	(kg/h)	8.358e+004 *	5.340e+004 *	2.505e+004 *	1.100e+005 *	1.390e+004 *
Std Ideal Liq Vol Flow	(m3/h)	279.2	764.4	31.34	133.3	13.93
Heat Flow	(kJ/h)	-3.440e+008	1.728e+008	-9.304e+007	-9.636e+008	-2.064e+008
Molar Enthalpy	(kJ/kgmole)	-6.604e+004	6523	-1.040e+005	-3.856e+005	-2.674e+005
Comp Mass Frac (CO)		0.0000 *	0.0000 *	1.0000 *	0.0000 *	0.0000 *
Comp Mass Frac (CO2)		0.0000 *	0.0000 *	0.0000 *	1.0000 *	0.0000 *
Comp Mass Frac (Hydrogen)		0.0000 *	1.0000 *	0.0000 *	0.0000 *	0.0000 *
Comp Mass Frac (H2O)		0.0000 *	0.0000 *	0.0000 *	0.0000 *	1.0000 *
Comp Mass Frac (Methanol)		0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Comp Mass Frac (Methane)		1.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *

Name		4-Vir	Duty MUG Comp	Duty Recycle Comp		
Vapour Fraction		1.0000	---	---		
Temperature	(C)	209.4	---	---		
Pressure	(kPa)	8000	---	---		
Molar Flow	(kgmole/h)	3.908e+004	---	---		
Mass Flow	(kg/h)	3.890e+005	---	---		
Std Ideal Liq Vol Flow	(m3/h)	1352	---	---		
Heat Flow	(kJ/h)	-2.079e+009	4.239e+007	1.697e+006		
Molar Enthalpy	(kJ/kgmole)	-5.319e+004	---	---		
Comp Mass Frac (CO)		0.0644	---	---		
Comp Mass Frac (CO2)		0.2827	---	---		
Comp Mass Frac (Hydrogen)		0.1373	---	---		
Comp Mass Frac (H2O)		0.0357	---	---		
Comp Mass Frac (Methanol)		0.2651	---	---		
Comp Mass Frac (Methane)		0.2148	---	---		

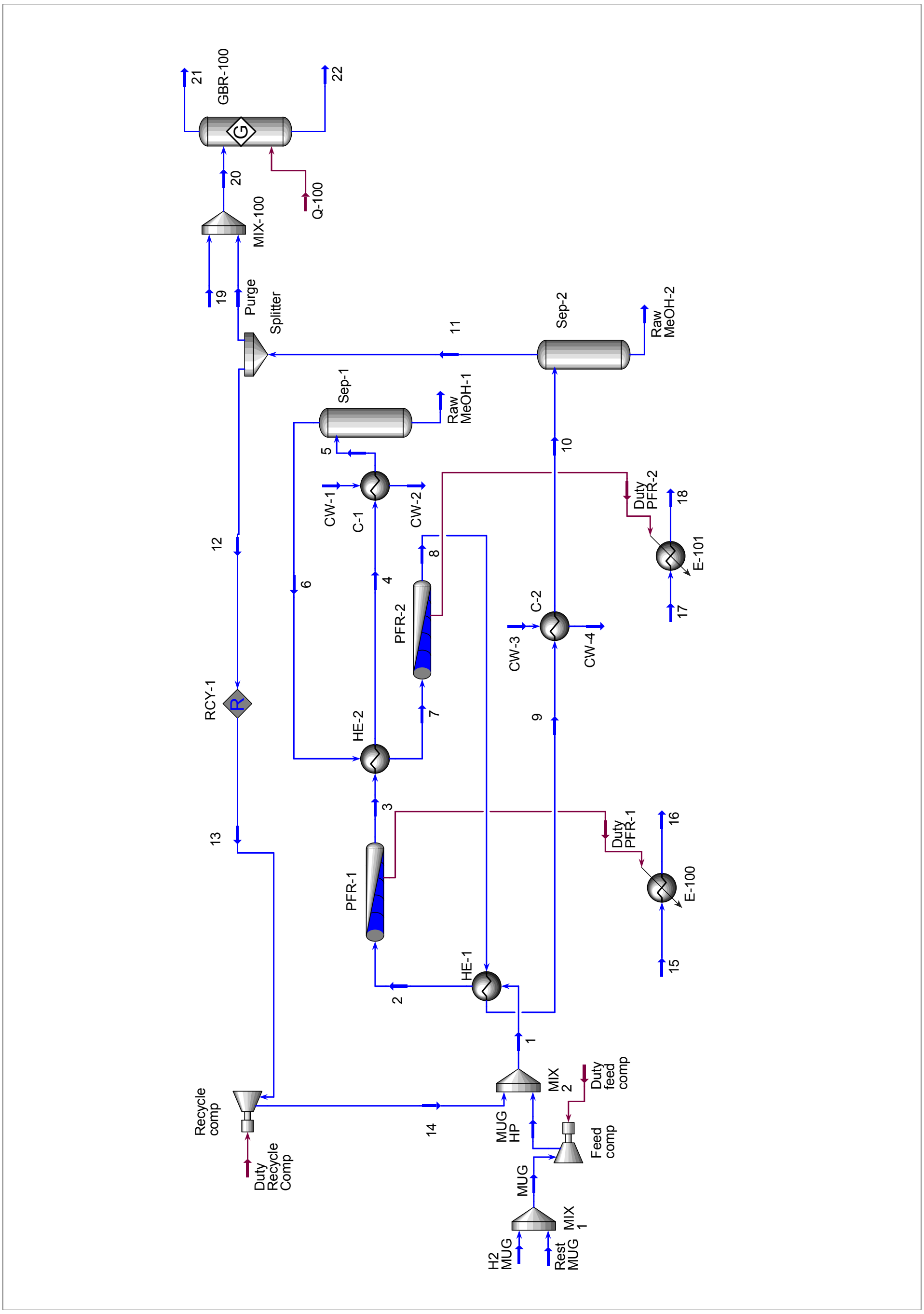
Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
MUG Comp	Compressor	MUG	1	No	500.0 *
		Duty MUG Comp			
Recycle Comp	Compressor	8	9	No	500.0 *
		Duty Recycle Comp			
MIX Recycle	Mixer	1	2	No	500.0 *
		9			
MIX MUG	Mixer	MUG others	MUG	No	500.0 *
		H2 MUG			
MIX-100	Mixer	MeOH	4-Vir	No	500.0 *
		CH4			
		H2			
		CO			
		CO2			
		H2O			

* Specified by user.

Appendix F

Interstage Methanol Removal


H2 MUG
Rest MUG
MIX 1
MUG
Feed comp
Duty feed comp
MUG HP
MIX 2
1
Recycle comp
Duty Recycle Comp
14
HE-1
2
PFR-1
3
Duty PFR-1
E-100
15
16
HE-2
7
PFR-2
8
4
C-1
CW-1
CW-2
5
Sep-1
Raw MeOH-1
6
13
RCY-1
R
12
Splitter
Purge
19
MIX-100
20
GBR-100
G
21
22
Q-100
11
Sep-2
Raw MeOH-2
10
9
C-2
CW-3
CW-4
Duty PFR-2
E-101
17
18

Company Name Not Available
Calgary, Alberta
CANADA

Case Name:	C:\Users\...\New Design\Interstage Methanol Removal.usc
Unit Set:	SI
Date/Time:	Friday Jun 3 2011, 15:07:11

Workbook: Case (Main)

Streams

Fluid Pkg: All

Name	Rest MUG	MUG HP	1	2	10
Vapour Fraction	0.9987	1.0000	1.0000	1.0000	0.9400
Temperature (C)	25.00 *	132.9	67.02	210.0 *	30.00
Pressure (kPa)	3000 *	8020 *	8020	8000	7611
Molar Flow (kgmole/h)	3498 *	1.132e+004	3.397e+004	3.397e+004	2.491e+004
Mass Flow (kg/h)	1.106e+005 *	1.264e+005	2.848e+005	2.848e+005	2.051e+005
Std Ideal Liq Vol Flow (m3/h)	142.8	368.6	1161	1161	869.8
Heat Flow (kJ/h)	-6.472e+008	-6.097e+008	-1.338e+009	-1.182e+009	-1.140e+009
Molar Enthalpy (kJ/kgmole)	-1.850e+005	-5.385e+004	-3.939e+004	-3.480e+004	-4.577e+004
Comp Mass Frac (CO)	0.6019 *	0.5268	0.2740	0.2740	0.0577
Comp Mass Frac (CO2)	0.3704 *	0.3242	0.2697	0.2697	0.1836
Comp Mass Frac (Hydrogen)	0.0000 *	0.1248	0.1733	0.1733	0.1693
Comp Mass Frac (H2O)	0.0016 *	0.0014	0.0009	0.0009	0.0412
Comp Mass Frac (Methanol)	0.0000 *	0.0000	0.0074	0.0074	0.1682
Comp Mass Frac (Methane)	0.0261 *	0.0228	0.2747	0.2747	0.3800
Comp Mass Frac (Oxygen)	0.0000 *	0.0000	0.0000	0.0000	0.0000

Name	Raw MeOH-2	11	Purge	14	12
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	30.00	30.00	30.00	35.19	30.00
Pressure (kPa)	7611	7611	7611	8020	7611
Molar Flow (kgmole/h)	1495	2.342e+004	769.9	2.265e+004	2.265e+004 *
Mass Flow (kg/h)	4.138e+004	1.637e+005	5384	1.584e+005	1.584e+005
Std Ideal Liq Vol Flow (m3/h)	50.05	819.7	26.95	792.8	792.8
Heat Flow (kJ/h)	-3.833e+008	-7.567e+008	-2.488e+007	-7.282e+008	-7.318e+008
Molar Enthalpy (kJ/kgmole)	-2.564e+005	-3.232e+004	-3.232e+004	-3.216e+004	-3.232e+004
Comp Mass Frac (CO)	0.0001	0.0723	0.0723	0.0723	0.0723
Comp Mass Frac (CO2)	0.0149	0.2262	0.2262	0.2262	0.2262
Comp Mass Frac (Hydrogen)	0.0002	0.2121	0.2121	0.2121	0.2121
Comp Mass Frac (H2O)	0.2022	0.0005	0.0005	0.0005	0.0005
Comp Mass Frac (Methanol)	0.7813	0.0132	0.0132	0.0132	0.0132
Comp Mass Frac (Methane)	0.0012	0.4758	0.4758	0.4758	0.4758
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000

Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

Name		9	13	H2 MUG	MUG	3
Vapour Fraction		0.9753	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	100.7	30.00 *	25.00 *	22.20	253.5
Pressure	(kPa)	7631	7611 *	3000 *	3000	7821
Molar Flow	(kgmole/h)	2.491e+004	2.265e+004 *	7825 *	1.132e+004	2.952e+004
Mass Flow	(kg/h)	2.051e+005	1.584e+005	1.578e+004	1.264e+005	2.848e+005
Std Ideal Liq Vol Flow	(m3/h)	869.8	792.8	225.8	368.6	1034
Heat Flow	(kJ/h)	-1.046e+009	-7.318e+008	-1.164e+004	-6.472e+008	-1.342e+009
Molar Enthalpy	(kJ/kgmole)	-4.200e+004	-3.232e+004	-1.488	-5.716e+004	-4.546e+004
Comp Mass Frac (CO)		0.0577	0.0723 *	0.0000 *	0.5268	0.0921
Comp Mass Frac (CO2)		0.1836	0.2262 *	0.0000 *	0.3242	0.2121
Comp Mass Frac (Hydrogen)		0.1693	0.2121 *	1.0000 *	0.1248	0.1392
Comp Mass Frac (H2O)		0.0412	0.0005 *	0.0000 *	0.0014	0.0245
Comp Mass Frac (Methanol)		0.1682	0.0132 *	0.0000 *	0.0000	0.2574
Comp Mass Frac (Methane)		0.3800	0.4758 *	0.0000 *	0.0228	0.2747
Comp Mass Frac (Oxygen)		0.0000	0.0000 *	0.0000 *	0.0000	0.0000

Name		4	Raw MeOH-1	6	7	8
Vapour Fraction		0.9680	0.0000	1.0000	1.0000	1.0000
Temperature	(C)	108.1	30.00	30.00	240.0 *	256.2
Pressure	(kPa)	7801	7781	7781	7761	7651
Molar Flow	(kgmole/h)	2.952e+004	2655	2.687e+004	2.687e+004	2.491e+004
Mass Flow	(kg/h)	2.848e+005	7.963e+004	2.051e+005	2.051e+005	2.051e+005
Std Ideal Liq Vol Flow	(m3/h)	1034	99.11	934.8	934.8	869.8
Heat Flow	(kJ/h)	-1.526e+009	-6.607e+008	-1.009e+009	-8.253e+008	-8.906e+008
Molar Enthalpy	(kJ/kgmole)	-5.167e+004	-2.488e+005	-3.754e+004	-3.071e+004	-3.575e+004
Comp Mass Frac (CO)		0.0921	0.0003	0.1278	0.1278	0.0577
Comp Mass Frac (CO2)		0.2121	0.0276	0.2837	0.2837	0.1836
Comp Mass Frac (Hydrogen)		0.1392	0.0003	0.1932	0.1932	0.1693
Comp Mass Frac (H2O)		0.0245	0.0870	0.0002	0.0002	0.0412
Comp Mass Frac (Methanol)		0.2574	0.8813	0.0152	0.0152	0.1682
Comp Mass Frac (Methane)		0.2747	0.0034	0.3800	0.3800	0.3800
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000

* Specified by user.

Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

Name		5	CW-2	CW-1	CW-3	CW-4
Vapour Fraction		0.9101	0.0000	0.0000	0.0000	0.0000
Temperature	(C)	30.00 *	50.00 *	15.00 *	15.00 *	50.00 *
Pressure	(kPa)	7781	80.00	100.0 *	100.0 *	80.00
Molar Flow	(kgmole/h)	2.952e+004	5.286e+004	5.286e+004	3.447e+004	3.447e+004
Mass Flow	(kg/h)	2.848e+005	9.522e+005	9.522e+005	6.209e+005	6.209e+005
Std Ideal Liq Vol Flow	(m3/h)	1034	954.2	954.2	622.2	622.2
Heat Flow	(kJ/h)	-1.669e+009	-1.503e+010	-1.517e+010	-9.892e+009	-9.798e+009
Molar Enthalpy	(kJ/kgmole)	-5.654e+004	-2.843e+005	-2.870e+005	-2.870e+005	-2.843e+005
Comp Mass Frac (CO)		0.0921	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (CO2)		0.2121	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (Hydrogen)		0.1392	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (H2O)		0.0245	1.0000	1.0000 *	1.0000 *	1.0000
Comp Mass Frac (Methanol)		0.2574	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (Methane)		0.2747	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Name		15	16	17	18	19
Vapour Fraction		0.0000 *	1.0000 *	0.0000 *	1.0000 *	1.0000
Temperature	(C)	250.0 *	250.0	255.0 *	255.0	30.00 *
Pressure	(kPa)	3913	3913	4250	4250	101.3 *
Molar Flow	(kgmole/h)	5077	5077	2104	2104	674.0 *
Mass Flow	(kg/h)	9.147e+004	9.147e+004	3.791e+004	3.791e+004	2.157e+004
Std Ideal Liq Vol Flow	(m3/h)	91.66	91.66	37.99	37.99	18.96
Heat Flow	(kJ/h)	-1.358e+009	-1.198e+009	-5.617e+008	-4.964e+008	9.212e+004
Molar Enthalpy	(kJ/kgmole)	-2.674e+005	-2.359e+005	-2.669e+005	-2.359e+005	136.7
Comp Mass Frac (CO)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (CO2)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (H2O)		1.0000 *	1.0000	1.0000 *	1.0000	0.0000 *
Comp Mass Frac (Methanol)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (Methane)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000 *	0.0000	0.0000 *	0.0000	1.0000 *

* Specified by user.

Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

Name		20	21	22	Duty feed comp	Duty Recycle Comp
Vapour Fraction		1.0000	1.0000	0.0000	---	---
Temperature	(C)	27.16	100.0	100.0 *	---	---
Pressure	(kPa)	101.3	101.3	101.3	---	---
Molar Flow	(kgmole/h)	1444	1155	0.0000	---	---
Mass Flow	(kg/h)	2.695e+004	2.695e+004	0.0000	---	---
Std Ideal Liq Vol Flow	(m3/h)	45.91	28.64	0.0000	---	---
Heat Flow	(kJ/h)	-2.479e+007	-2.925e+008	0.0000	3.752e+007	3.588e+006
Molar Enthalpy	(kJ/kgmole)	-1.717e+004	-2.532e+005	-2.804e+005	---	---
Comp Mass Frac (CO)		0.0144	0.0000	0.0000	---	---
Comp Mass Frac (CO2)		0.0452	0.3322	0.0001	---	---
Comp Mass Frac (Hydrogen)		0.0424	0.0000	0.0000	---	---
Comp Mass Frac (H2O)		0.0001	0.5951	0.9999	---	---
Comp Mass Frac (Methanol)		0.0026	0.0000	0.0000	---	---
Comp Mass Frac (Methane)		0.0950	0.0000	0.0000	---	---
Comp Mass Frac (Oxygen)		0.8002	0.0727	0.0000	---	---

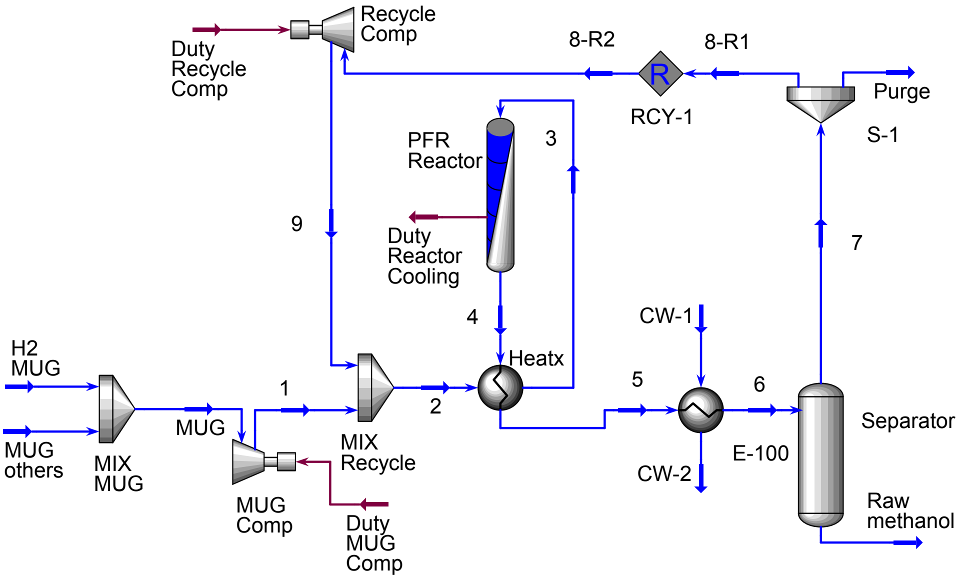
Name		Duty PFR-2	Duty PFR-1	Q-100		
Vapour Fraction		---	---	---		
Temperature	(C)	---	---	---		
Pressure	(kPa)	---	---	---		
Molar Flow	(kgmole/h)	---	---	---		
Mass Flow	(kg/h)	---	---	---		
Std Ideal Liq Vol Flow	(m3/h)	---	---	---		
Heat Flow	(kJ/h)	6.528e+007	1.599e+008	-2.677e+008		
Molar Enthalpy	(kJ/kgmole)	---	---	---		
Comp Mass Frac (CO)		---	---	---		
Comp Mass Frac (CO2)		---	---	---		
Comp Mass Frac (Hydrogen)		---	---	---		
Comp Mass Frac (H2O)		---	---	---		
Comp Mass Frac (Methanol)		---	---	---		
Comp Mass Frac (Methane)		---	---	---		
Comp Mass Frac (Oxygen)		---	---	---		

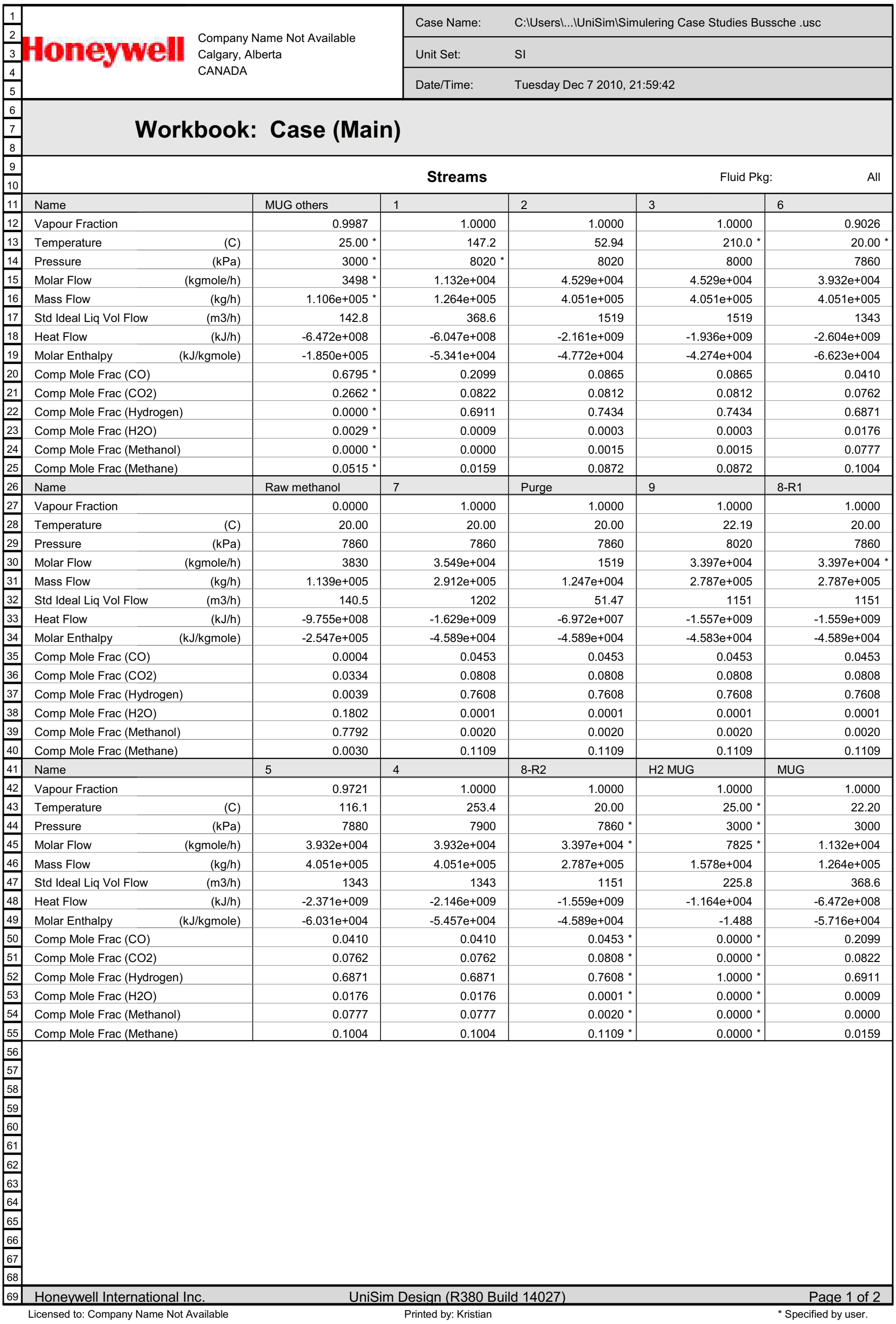
Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
Feed comp	Compressor	MUG Duty feed comp	MUG HP	No	500.0 *
Recycle comp	Compressor	13 Duty Recycle Comp	14	No	500.0 *
MIX 2	Mixer	MUG HP 14	1	No	500.0 *
MIX 1	Mixer	Rest MUG H2 MUG	MUG	No	500.0 *
MIX-100	Mixer	Purge 19	20	No	500.0 *
PFR-1	Plug Flow Reactor	2	3 Duty PFR-1	No	500.0 *

Appendix G

UniSim Base Case





Honeywell

Company Name Not Available
Calgary, Alberta
CANADA

Case Name:	C:\Users\...\UniSim\Simulering Case Studies Bussche .usc
Unit Set:	SI
Date/Time:	Tuesday Dec 7 2010, 21:59:42

Workbook: Case (Main)

Streams

Fluid Pkg: All

Name		MUG others	1	2	3	6
Vapour Fraction		0.9987	1.0000	1.0000	1.0000	0.9026
Temperature	(C)	25.00 *	147.2	52.94	210.0 *	20.00 *
Pressure	(kPa)	3000 *	8020 *	8020	8000	7860
Molar Flow	(kgmole/h)	3498 *	1.132e+004	4.529e+004	4.529e+004	3.932e+004
Mass Flow	(kg/h)	1.106e+005 *	1.264e+005	4.051e+005	4.051e+005	4.051e+005
Std Ideal Liq Vol Flow	(m3/h)	142.8	368.6	1519	1519	1343
Heat Flow	(kJ/h)	-6.472e+008	-6.047e+008	-2.161e+009	-1.936e+009	-2.604e+009
Molar Enthalpy	(kJ/kgmole)	-1.850e+005	-5.341e+004	-4.772e+004	-4.274e+004	-6.623e+004
Comp Mole Frac (CO)		0.6795 *	0.2099	0.0865	0.0865	0.0410
Comp Mole Frac (CO2)		0.2662 *	0.0822	0.0812	0.0812	0.0762
Comp Mole Frac (Hydrogen)		0.0000 *	0.6911	0.7434	0.7434	0.6871
Comp Mole Frac (H2O)		0.0029 *	0.0009	0.0003	0.0003	0.0176
Comp Mole Frac (Methanol)		0.0000 *	0.0000	0.0015	0.0015	0.0777
Comp Mole Frac (Methane)		0.0515 *	0.0159	0.0872	0.0872	0.1004

Name		Raw methanol	7	Purge	9	8-R1
Vapour Fraction		0.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	20.00	20.00	20.00	22.19	20.00
Pressure	(kPa)	7860	7860	7860	8020	7860
Molar Flow	(kgmole/h)	3830	3.549e+004	1519	3.397e+004	3.397e+004 *
Mass Flow	(kg/h)	1.139e+005	2.912e+005	1.247e+004	2.787e+005	2.787e+005
Std Ideal Liq Vol Flow	(m3/h)	140.5	1202	51.47	1151	1151
Heat Flow	(kJ/h)	-9.755e+008	-1.629e+009	-6.972e+007	-1.557e+009	-1.559e+009
Molar Enthalpy	(kJ/kgmole)	-2.547e+005	-4.589e+004	-4.589e+004	-4.583e+004	-4.589e+004
Comp Mole Frac (CO)		0.0004	0.0453	0.0453	0.0453	0.0453
Comp Mole Frac (CO2)		0.0334	0.0808	0.0808	0.0808	0.0808
Comp Mole Frac (Hydrogen)		0.0039	0.7608	0.7608	0.7608	0.7608
Comp Mole Frac (H2O)		0.1802	0.0001	0.0001	0.0001	0.0001
Comp Mole Frac (Methanol)		0.7792	0.0020	0.0020	0.0020	0.0020
Comp Mole Frac (Methane)		0.0030	0.1109	0.1109	0.1109	0.1109

Name		5	4	8-R2	H2 MUG	MUG
Vapour Fraction		0.9721	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	116.1	253.4	20.00	25.00 *	22.20
Pressure	(kPa)	7880	7900	7860 *	3000 *	3000
Molar Flow	(kgmole/h)	3.932e+004	3.932e+004	3.397e+004 *	7825 *	1.132e+004
Mass Flow	(kg/h)	4.051e+005	4.051e+005	2.787e+005	1.578e+004	1.264e+005
Std Ideal Liq Vol Flow	(m3/h)	1343	1343	1151	225.8	368.6
Heat Flow	(kJ/h)	-2.371e+009	-2.146e+009	-1.559e+009	-1.164e+004	-6.472e+008
Molar Enthalpy	(kJ/kgmole)	-6.031e+004	-5.457e+004	-4.589e+004	-1.488	-5.716e+004
Comp Mole Frac (CO)		0.0410	0.0410	0.0453 *	0.0000 *	0.2099
Comp Mole Frac (CO2)		0.0762	0.0762	0.0808 *	0.0000 *	0.0822
Comp Mole Frac (Hydrogen)		0.6871	0.6871	0.7608 *	1.0000 *	0.6911
Comp Mole Frac (H2O)		0.0176	0.0176	0.0001 *	0.0000 *	0.0009
Comp Mole Frac (Methanol)		0.0777	0.0777	0.0020 *	0.0000 *	0.0000
Comp Mole Frac (Methane)		0.1004	0.1004	0.1109 *	0.0000 *	0.0159

Honeywell International Inc. UniSim Design (R380 Build 14027) Page 1 of 2

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Honeywell
Company Name Not Available
Calgary, Alberta
CANADA

Case Name:	C:\Users\...\UniSim\Simulering Case Studies Bussche .usc
Unit Set:	SI
Date/Time:	Tuesday Dec 7 2010, 21:59:42

Workbook: Case (Main) (continued)

Streams (continued)

Fluid Pkg: All

Name	Duty Reactor Cooling	Duty Condenser	Duty MUG Comp	Duty Recycle Comp	
Vapour Fraction	---	---	---	---	
Temperature (C)	---	---	---	---	
Pressure (kPa)	---	---	---	---	
Molar Flow (kgmole/h)	---	---	---	---	
Mass Flow (kg/h)	---	---	---	---	
Std Ideal Liq Vol Flow (m3/h)	---	---	---	---	
Heat Flow (kJ/h)	2.098e+008	2.329e+008 *	4.252e+007 *	2.254e+006 *	
Molar Enthalpy (kJ/kgmole)	---	---	---	---	
Comp Mole Frac (CO)	---	---	---	---	
Comp Mole Frac (CO2)	---	---	---	---	
Comp Mole Frac (Hydrogen)	---	---	---	---	
Comp Mole Frac (H2O)	---	---	---	---	
Comp Mole Frac (Methanol)	---	---	---	---	
Comp Mole Frac (Methane)	---	---	---	---	

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
MUG Comp	Compressor	MUG Duty MUG Comp	1	No	500.0 *
Recycle Comp	Compressor	8-R2 Duty Recycle Comp	9	No	500.0 *
MIX Recycle	Mixer	1 9	2	No	500.0 *
MIX MUG	Mixer	MUG others H2 MUG	MUG	No	500.0 *
PFR Reactor	Plug Flow Reactor	3	4 Duty Reactor Cooling	No	500.0 *
Condenser	Cooler	5	6 Duty Condenser	No	500.0 *
Separator	Separator	6	Raw methanol 7	No	500.0 *
S-1	Tee	7	Purge 8-R1	No	500.0 *
Heatx	Heat Exchanger	4 2	5 3	No	500.0 *
Parameters	Spreadsheet			No	500.0 *
Massebal	Spreadsheet			No	500.0 *
Compressor	Spreadsheet			No	500.0 *
ADJ-UA	Adjust			No	3500 *
RCY-1	Recycle	8-R1	8-R2	No	3500 *

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Appendix H

Pinch Analysis

To find the optimum configuration for the heat exchanger network, a pinch analysis was conducted (Gundersen, 2001). A pinch analysis is based on composite curves for the hot and cold streams in the facility, and uses these to find the pinch point in the process. Table H.1 and Table H.2 is generated from the values obtained from the simulation shown in Figure H.1.

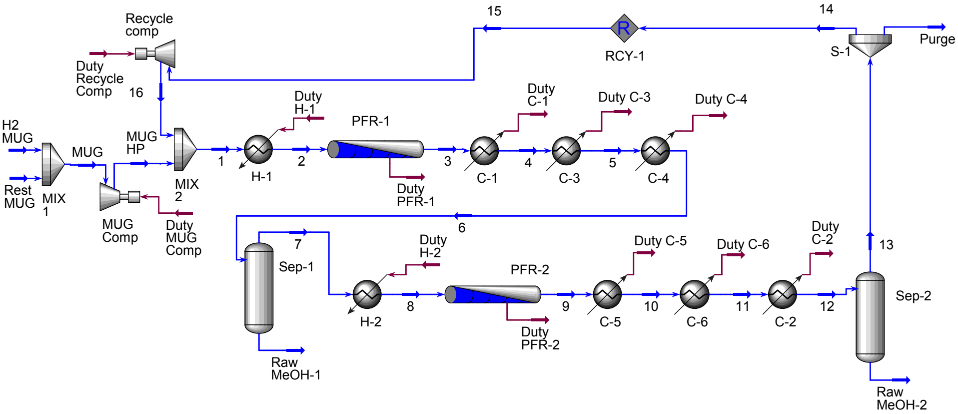


Figure H.1: UniSim layout

Since methanol and water is condensing it was desirable to divide the condenser into three parts since the C_p values changes drastically when the stream is condensed.

Table H.1: Data for the hot curve

Stream to	Temp. interval [°C]		$\dot{m}C_p$	Q [kJ t^{-1}]	Q$_{tot}$
Sep-2	256	255	865 685	865 685	865 685
Sep-1	255	126	1 039 969	134 156 054	
Sep-2	255	126	865 685	111 673 374	245 829 428
Sep-1	126	122	2 670 631	10 682 524	
Sep-2	126	122	865 685	3 462 740	14 145 265
Sep-1	122	100	2 670 631	58 753 883	
Sep-2	122	100	1 858 937	40 896 615	99 650 499
Sep-1	100	30	1 767 181	123 702 674	
Sep-2	100	30	1 323 105	92 617 348	216 320 023

Table H.2: Data for the cold curve

Stream to	Temp. interval [°C]		$\dot{m}C_p$	Q [kJ t^{-1}]	Q$_{tot}$
PFR-1	30	67	873 638	32 324 620	32 324 620
PFR-2	67	210	873 638	124 930 287	
PFR-1	67	210	1 088 923	155 715 974	280 646 261
PFR-2	210	240	873 638	26 209 151	26 209 151

The composition curves were drawn from the data in Table H.1 and Table H.2, and can be seen in Figure 4.14. To localize the pinch point the cold curve was moved to the right. This is valid because it is the enthalpy change, and not the absolute value of the enthalpy that is of interest.

Appendix I

Economy

To find the price of the various equipment the following formula was used:

$$C_e = a + bS^n$$

Where C_e is the equipment price, S is a caracteristic size and a, b and n are constants from Table 6.6 is Sinnott and Towler (2009).

S for the separators was the shell mass. To find this mass the design procedure on page 638 in Sinnott and Towler (2009) was used.

Index oct 2010	**556,30**	
Pressure factor	**1,30**	
Base case separator		
Rho liq	809,53	kg/m3
Rho vap	23,82	kg/m3
Setteling velocity	0,40	Ut m/s
Vapour flow rate	3,15	m3/s Vv
Liquid flow rate m3/h	145,87	m3/h Vl
Dmin	**3,16**	
H liq	**3,10**	10 min recidense time
Hmin	8,24	
Wall thickness	0,166	tw m
Metal density	8 000	kg/m3
Shell mass	108 799	
Price oct 10	615 593	$

Two PFR

Sep 1

Rho liq	799,99	kg/m3
Rho vap	23,31	kg/m3
Setteling velocity	0,40	Ut m/s
Vapour flow rate	2,45	m3/s Vv
Liquid flow rate m3/h	99,54	m3/h Vl
Dmin	2,78	
H liq	2,74	10 min recidense time
Hmin	7,31	
Wall thickness	0,15	tw m
Metal density	8 000	kg/m3
Shell mass	74 387	
Price oct 10	448 602	$

Sep 2

Rho liq	823,29	kg/m3
Rho vap	20,87	kg/m3
Setteling velocity	0,43	Ut m/s
Vapour flow rate	2,18	m3/s Vv
Liquid flow rate m3/h	50,26	m3/h Vl
Dmin	2,53	
H liq	1,67	10 min recidense time
Hmin	5,86	
Wall thickness	0,133	tw m
Metal density	8 000,00	kg/m3
Shell mass	49 529	
Price oct 10	320 671	$

Two PFR Sep cost	**769 273,04**	$

Heatx

	Base Case	Two PFR		
UA	4 314 837	3 931 435	4 980 409	kJ C^-1 h^-1
UA	1 198 566	1 092 065	1 383 447	W K^-1
U	500	500	500	W m^2 K
A	2 397	2 184	2 767	m^2
Price oct 10	697 685	634 763	809 553	$
Price oct 10	**697 685**	**1 444 316**		$

Condenser

	Base Case	Two PFR		
UA	6 492 032	4 519 566	3 199 870	kJ/(C*h)
UA	1 803 342	1 255 435	888 853	W K^-1
U	600	600	600	W m^2 K
A	3 006	2 092	1 481	m^2
Price oct 10	883 396	608 032	436 419	$
Price oct 10	**883 396**	**1 044 451**		$

Recycle Comp

	Base Case	Two PFR		
Duty	572	997	kW	
Price oct 10	**161 824**	**222 222**	$	
Op Price oct 10	**23**	**39**	**$ /h**	22 øre/kWh

Methanol prod

	Base Case	Two PFR		
MeOH prod	99 705	102 510	kg h^-1	
Income	**32 404**	**33 316**	€ h^-1	325 €/MT
Income	**45 560**	**46 842**	$/h	

Purge

	Base Case	Two PFR		
Purge heat flow	-334 562 988	-292 451 788	kJ h^-1	
Purge heat flow	**335**	**292**	GJ h^-1	
Income	**1 338**	**1 170**	$/h	4 $/GJ

MP steam

	Base Case	Two PFR		
Steam	126 798	129 381	kg h^-1	
Income	**1 522**	**1 553**	$/h	12 $/MT

Investment cost

		Base Case	Two PFR	Installation
Purchased cost	Sep cost	615 593	769 273	4
	Heat exchanger cost	697 685	1 444 316	3,5
	Condenser cost	883 396	1 044 451	3,5
	Recycle comp cost	161 824	222 222	2,5
	Sum	2 358 498	3 480 262	
Installed cost	Sep cost	2 462 371	3 077 092	
	Heat exchanger cost	2 441 897	5 055 107	
	Condenser cost	3 091 886	3 655 577	
	Recycle comp cost	404 560	555 556	
	Sum	8 400 714	12 343 332	

Operating cost

	Base Case	Two PFR	
Recycle comp	177 861	310 009	$ / year

Income

	Base Case	Two PFR	
Methanol	364 480 211	374 736 345	$ / year
Purge	10 706 016	9 358 457	$ / year
MP steam	12 172 652	12 420 597	$ / year
	387 358 879	396 515 399	$ / year

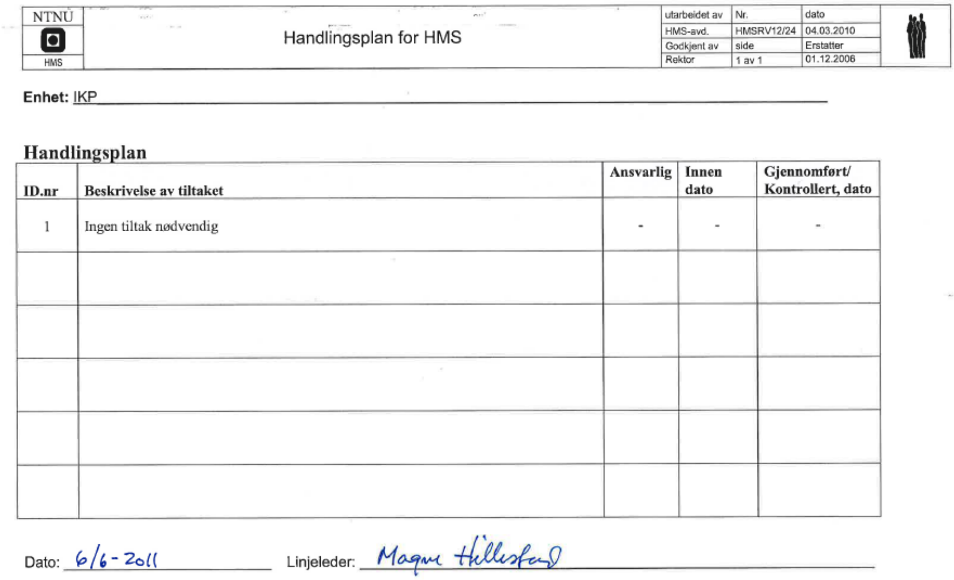
	Base Case	Two PFR	Difference	Unit
Investment cost	8 400 714	12 343 332	3 942 618	$
Operating cost	177 861	310 009	132 148	$/year
Income	387 358 879	396 515 399	9 156 520	$/year

All values are in 1000$

	Basis	-1	0	1	2	3	4	5	6	7	8	9	10
Fixed capital investment	3 943												
Working capital													
Declining balance 20 %	20												
Depreciation factor		a*(1-a)^(i-1)		0,2	0,1600	0,1280	0,1024	0,0819	0,0655	0,0524	0,0419	0,0336	0,0268
Fixed investment			-3942,6										
Working capital			0										
Return of working capital													0
Annual Operating revenue	9 157			9157	9157	9157	9157	9157	9157	9157	9157	9157	9157
Annual operating costs, fixed	0			132	132	132	132	132	132	132	132	132	132
Annual operating costs, variable	132												
Total annual operating costs	132												
Gross operating result				9024	9024	9024	9024	9024	9024	9024	9024	9024	9024
Depreciation				789	631	505	404	323	258	207	165	132	106
Pre tax results				8236	8394	8520	8621	8701	8766	8818	8859	8892	8919
Tax, percentage 28%	28			2306	2350	2386	2414	2436	2454	2469	2481	2490	2497
Net profit				5930	6043	6134	6207	6265	6312	6349	6378	6402	6421
Amortisation				789	631	505	404	323	258	207	165	132	106
Net cash flow			-3942,6	6718	6674	6639	6611	6588	6570	6555	6544	6535	6527
Accumulated NCF (Net cash flow)		0	-3942,6	2776	9450	16089	22699	29287	35857	42413	48956	55491	62018
Rate of interest (%)	5,00		1,00	0,95	0,91	0,86	0,82	0,78	0,75	0,71	0,68	0,64	0,61
Discounted NCF		0	-3942,6	6398	6054	5735	5439	5162	4903	4659	4429	4212	4007
Accumulated discounted NCF			-3942,6	2456	8509	14244	19683	24845	29747	34406	38835	43048	47055
Internal interest	**5,0**												
Net present worth (NPV)	**47055**												

Appendix J

HSE



NTNU
HMS

Handlingsplan for HMS

utarbeidet av	Nr.	dato
HMS-avd.	HMSRV12/24	04.03.2010
Godkjent av	side	Erstatter
Rektor	1 av 1	01.12.2006

Enhet: IKP

Handlingsplan

ID.nr	Beskrivelse av tiltaket	Ansvarlig	Innen dato	Gjennomført/ Kontrollert, dato
1	Ingen tiltak nødvendig	-	-	-

Dato: 6/6-2011 Linjeleder: Magne Hillestad

NTNU	Kartlegging av risikofylt aktivitet	Utarbeidet av	Nummer	Dato
		HMS-avd.	HMSRV2601	05.03.2010
		Godkjent av	Side	Erstatter
HMS		Rektor	1 av 2	01.12.2006

Enhet: IKP

Dato: 06.06.2011

Deltakere ved kartleggingen (m/ funksjon):
Kristian Bøhn (Utførende)

Kort beskrivelse av hovedaktivitet/hovedprosess:
Datasimulering kun på lesesal

ID nr.	Aktivitet/prosess	Ansvarlig	Lov, forskrift o.l.	Eksisterende dokumentasjon	Eksisterende sikringstiltak	Kommentar
1	Datasimulering	-	-	NTNU HMS håndbok	-	Ingen risiko

NTNU	Kartlegging av risikofylt aktivitet	Utarbeidet av	Nummer	Dato
		HMS-avd.	HMSRV2601	05.03.2010
		Godkjent av	Side	Erstatter
HMS		Rektor	2 av 2	01.12.2006

Hva

Aktivitet/prosess
Kartlegging av aktiviteter/prosesser som inngår i risikovurderingen og som kan inneha risiko for skade på menneske eller miljø. Dette kan f.eks. være maskiner, labaktivitet, verkstedarbeid, bruk av visse kjemikalier osv. Bryt ned hele aktiviteten/prosessen i enkeltdeler, beskriv kort hver del.

Aktivitetene velges enten som gjennomgang av en prosess (aktivitet fra f.eks. innkjøp av materiale, via bearbeiding til ferdig produkt), eller alle aktiviteter som oppleves mulig risikofylte i et gitt område. Deltagerne må bli enige om omfanget av aktivitetene som skal risikovurderes,

Man må ta stilling til
- "Risiko for hvem" - for ansatte, for nabomiljø, for enkeltindivider eller en gruppe, for bedriften, for samfunnet
- "Risiko fra hva" - hvilket anlegg, hvilken aktivitet, fra hvilke ulykkeskategorier
- "For hvilket tidsrom"- risikonivået kan variere over tid

Risiko er et potensielt tap, ikke et oppstått tap. Aktiviteter/prosesser som i utgangspunktet blir vurdert som lite risikofylte, kan medføre økt risiko under gitte forhold.

Ansvarlig
Hvem er ansvarlig for de enkelte aktiviteter/prosesser? Er det noen andre enheter som har ansvar eller oppgaver for å redusere risiko? Organisasjonskart kan brukes for å avklare ansvarsforhold

Lov, forskrift o.l.
Hvilke lover, forskrifter og andre myndighetskrav gjelder for aktiviteten/prosessen? Se HMS-håndboka, HMSRV-20/01, www.lovdata.no, www.arbeidstilsynet.no, www.hmsetatene.no, kommunale bestemmelser (www.trondheim.kommune.no)

Eksisterende dokumentasjon
Enheten skal finne fram eksisterende sentrale og lokale retningslinjer, tegningsunderlag, sertifikater, kranførerbevis, truckførerbevis, gjennomført opplæring, serviceavtaler, bruksanvisninger, sjekklister osv. Se også tidligere risikovurderinger og HMS-runder, lokalt HMS-hefte, labhåndbok, NTNUs stoffkartotek osv.

Sikringstiltak
Hva finnes av eksisterende sikringstiltak for området/utstyret? Feks. ventilasjon, personlig verneutstyr, nødstopp, merking/ilting, skillevegger osv.

NTNU	Risikovurdering	utarbeidet av	Nummer	Dato
		HMS-avd.	HMSRV2603	4.3.2010
		godkjent av	side	Erstatter
HMS/KS		Rektor	1 av 2	9.2.2010

Enhet:IKP **Dato:** 06.06.2011
Linjeleder: Professor Magne Hillestad
Deltakere ved risikovurderingen (m/ funksjon): Kristian Bøhn

	Aktivitet fra kartleggings-skjemaet	**Mulig uønsket hendelse/ belastning**	**Vurdering av sannsyn-lighet**	**Vurdering av konsekvens:**				**Risiko-verdi**	**Kommentarer/status Forslag til tiltak**
ID nr			(1-5)	Menneske (A-E)	Ytre miljø (A-E)	Øk/ materiell (A-E)	Om-dømme (A-E)		
1	Datasimulering	Ingen	-	-	-	-	-	-	Ingen risiko knyttet til oppgaven

Sannsynlighet
1. Svært liten
2. Liten
3. Middels
4. Stor
5. Svært stor

Konsekvens
A. Svært liten
B. Liten
C. Moderat
D. Alvorlig
E. Svært alvorlig

Risikoverdi (beregnes hver for seg):
Menneske = Sannsynlighet x Konsekvens Menneske
Ytre miljø = Sannsynlighet x Konsekvens Ytre miljø
Økonomi/materiell = Sannsynlighet x Konsekvens Øk/matriell
Omdømme = Sannsynlighet x Konsekvens Omdømme

Sannsynlighet vurderes etter følgende kriterier:

Svært liten 1	Liten 2	Middels 3	Stor 4	Svært stor 5
1 gang pr 50 år eller sjeldnere	1 gang pr 10 år eller sjeldnere	1 gang pr år eller sjeldnere	1 gang pr måned eller oftere	Skjer ukentlig

Konsekvens vurderes etter følgende kriterier:

Gradering	Menneske	Ytre miljø Vann, jord og luft	Øk/materiell	Omdømme
E Svært Alvorlig	Død	Svært langvarig og ikke reversibel skade	Drifts- eller aktivitetsstans >1 år.	Troverdighet og respekt betydelig og varig svekket
D Alvorlig	Alvorlig personskade. Mulig uførhet.	Langvarig skade. Lang restitusjonstid	Driftsstans > ½ år Aktivitetsstans i opp til 1 år	Troverdighet og respekt betydelig svekket
C Moderat	Alvorlig personskade.	Mindre skade og lang restitusjonstid	Drifts- eller aktivitetsstans < 1 mnd	Troverdighet og respekt svekket
B Liten	Skade som krever medisinsk behandling	Mindre skade og kort restitusjonstid	Drifts- eller aktivitetsstans < 1uke	Negativ påvirkning på troverdighet og respekt
A Svært liten	Skade som krever førstehjelp	Ubetydelig skade og kort restitusjonstid	Drifts- eller aktivitetsstans < 1dag	Liten påvirkning på troverdighet og respekt

Risikoverdi = Sannsynlighet x Konsekvens
Beregn risikoverdi for Menneske. Enheten vurderer selv om de i tillegg vil beregne risikoverdi for Ytre miljø, Økonomi/materiell og Omdømme. I så fall beregnes disse hver for seg.

Til kolonnen ”Kommentarer/status, forslag til forebyggende og korrigerende tiltak”:
Tiltak kan påvirke både sannsynlighet og konsekvens. Prioriter tiltak som kan forhindre at hendelsen inntreffer, dvs. sannsynlighetsreduserende tiltak foran skjerpet beredskap, dvs. konsekvensreduserende tiltak.