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Methanol Synthesis Process
using an autothermal rod-bundle reformer

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Summary

A methanol plant was developed for the production of 380,000 metric tons (12.07 kg/s) per year. The goal of 350,000 metric tons is reached. The methanol is 98,8 % pure. The impurity was mainly caused by dimethylether which is difficult to remove.

The reformer is operated autothermal, which was one of the goals of this assignment. The autothermal process is achieved due to intensive heat integration. As a result the plant has ~~a lot of~~ large heat exchangers.

The investment costs of the plant are fl. 100 million (rough estimation). The sales income of the methanol depends strongly on the methanol price used. Using the price according to Coulson the methanol sales income is fl. 735 million per year. This would mean that the investment is earned back within one year. The plant is very profitable. Using the price according to Calis the methanol sales income will be fl. 94.5 million , the net cash flow becomes below zero and the process is not profitable. No clear view of the economics is gained.

The natural gas cleaning is not included in the design.

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Introduction

The assignment was to develop a process for the production of 350,000 metric tons of methanol per year. Natural gas is used as base material. The methane is converted in an autothermal reformer into synthesis gas. The reformer is a rodd bundle reactor, the catalyst hangs in bundles in the reformer. This concept is very new, so there is little known on the kinetics of the reactor.

The synthesis is converted into methane in a packed bed reactor. The kinetics of this is well known. The heat produced in the reactor is used to preheat the natural gas. Therefore the reactor contents four packed beds of different sizes. The catalyst used is the well known MK101 which has a selectivity of 99%.

The main goal is to design the autothermal reformer. To make it autothermal one third of the natural gas is burned with pure oxygen. The rest of the gas is reformed with steam. The advantage is not only savings in energy costs but also the outlet of the reactor is stoechiometric. Therefore less hydrogen is wasted then in former reformer processes.

Also the economical aspects of the methanol process are calculated.

Methanol is one of the most used base materials in the world. The world production is 12 mega tons per year. In western Europe 4 MT are produced, in Holland 0.7 MT are produced, this is caused by the natural gas fields in Groningen.

Methanol is used as:

* base material for methanal production,
* intermediate for ester reactions,
* solvent,
* base material for acetic acid,
* fuel for motors.

Disadvantages of methanol are the toxicity, the flammability and the environmental pollution. Methanol has similarities with ethanol (alcohol),it has a same taste, odor and you can get drunk of it. Many people died or got blind after drinking methanol.

Because methanol is very flammable it can form explosive gas with air. Production and storage comply with many safety restrictions.

The production of methanol causes no environmental pollution. Also the use as base chemical causes no pollution. The use as fuel does cause environmental pollution, almost as much CO and CO_2 as normal gasoline but also methanal is found in the exhaust gasses. Methanal is very environmental aggravating.

Chapter 1 Basic Assumptions

1.1 Process bloc scheme.

In figure I a bloc scheme of the methanol production is shown. This route for the production of methanol is well known and often used. The cleaning of the natural gas is not included in this design. It is assumed that enough cleaning techniques are developed which are suitable and available for this process.

The natural gas is partial burned in the reformer. The heat which is released is used to convert the natural gas into synthesis gas ($CO+H_2$). This way the reformer operates autothermal. After cooling the excess water is removed. After compressing the synthesis gas enters the synthesis reactor. The synthesis gas is converted into methanol, a recycle flow increases the conversion. Finally the methanol is purified.

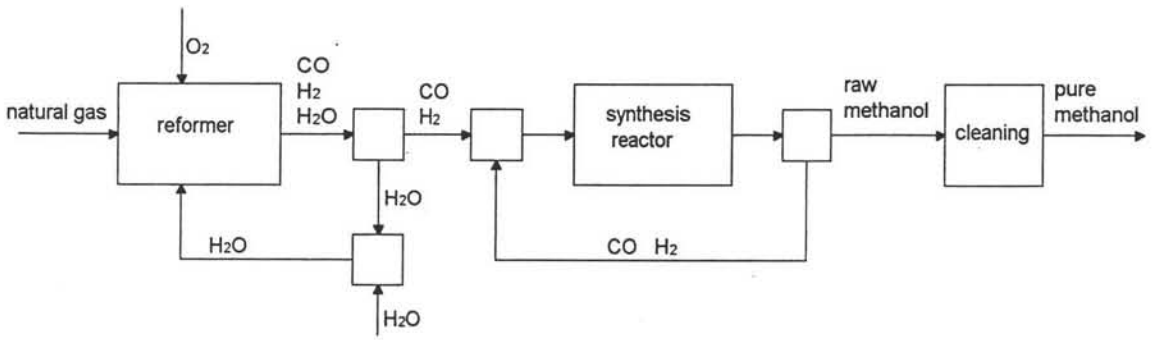


figure 1 Bloc scheme of the methanol synthesis

1.2 Reactions

The two most important reactions which occur in the reformer:

$$CH_4 + H_2O \longleftrightarrow CO + 3H_2 \qquad (1)$$

$$\Delta H_{298K} = 205.8 \text{ kJ / mol}$$

$$CH_4 + O_2 \longleftrightarrow CO + H_2O + H_2 \qquad (2)$$

$$\Delta H_{298K} = -277.8 \text{ kJ / mol}$$

overall reactie is :

$$CH_4 + \frac{1}{2} O_2 \longleftrightarrow CO + 2H_2 \qquad (3)$$

In the reformer the following three reactions take place:

$$CO + 2H_2 \longleftrightarrow CH_3OH \qquad (4)$$

$$\Delta H_{300K} = -90.77 \text{ kJ / mol}$$

$$CO_2 + H_2 \longleftrightarrow CO + H_2O \qquad (5)$$

$$\Delta H_{300K} = 41.21 \text{ kJ / mol}$$

$$CO_2 + 3H_2 \longleftrightarrow CH_3OH + H_2O \qquad (6)$$

$$\Delta H_{300K} = -49.16 \text{ kJ / mol}$$

The first one represents the overall-reaction; the other two only influence conversion-degrees and reaction rates.

1.3 General process figures

For the location the province Noord-Holland in the Netherlands is chosen. This because in this design North sea gas is used. This gas has the following composition:

table 1 composition of North Sea gas:

	[%]
methane	95
ethane	2.9
propane	0.5
butane	0.2
nitrogen	1.2
other	0.2

For further calculations a composition of 98.8% methane and 1.2% nitrogen is used.
It is assumed that the gas is cleaned of catalysts poisoning compounds like sulphur.
The produced methanol must have a purity of 98.5%.
River water is used for cooling purposes and may be heated from 20°C to 40 °C .

Chapter 2 Process structure

2.1 Process conditions and justifications

The temperature in the reformer is restricted to the range of 900 to 1050 K.
In this range the equilibrium is in favour of synthesis gas.
Below 900 K the rate of the reaction between steam and methane is to small; above 1050 K there will be too much carbon deposition, which will deactivate the catalyst.

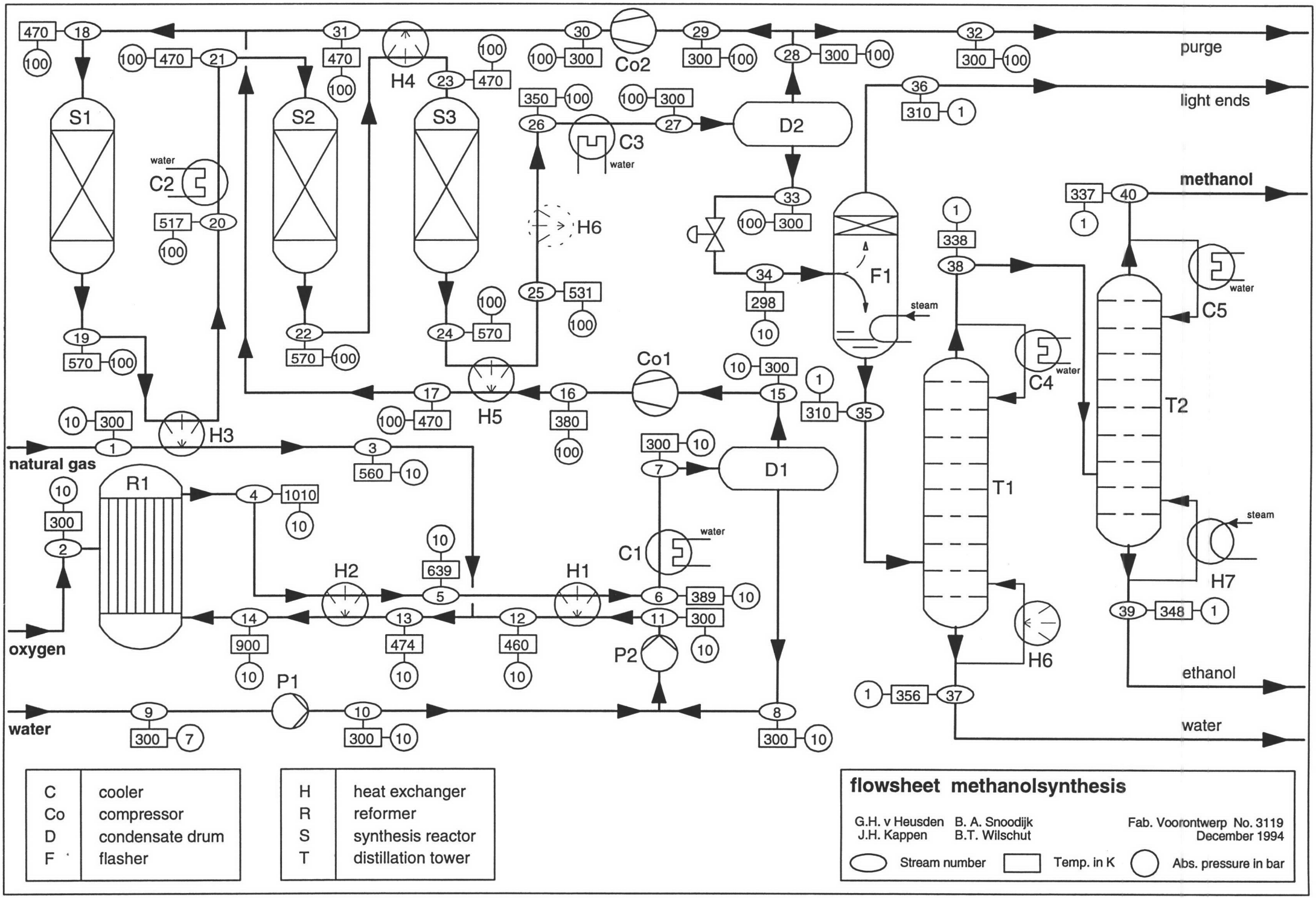
There are three oxygen injections in the reformer to maintain this restriction.
The exothermic reaction of oxygen with methane provides the energy for the endothermic reaction of steam with methane.

A low pressure favours the equilibrium, but since kinetics involves the partial pressure of methane it lowers the reaction rate. A pressure of ten bar was part of the assignment.

A steam recycle in ratio steam : methane of 5:1 is chosen. This favours the equilibrium and prevents carbon deposition. Unfortunately this drives up the operation costs of the reformer.

A temperature range in the synthesis reactor of 470 to 570 K is recommended in the literature, because in this range no phase transition takes place an all reaction rates and selectivity's are in favour of the synthesis of methanol. Equilibrium does not allow conversion ratios higher than about 50% ; therefore a recycle is implemented.
Because of improved catalysts the methanol synthesis can nowadays be carried out at pressures as low as 100 bar. This used to be 250 bar or more.

Because the methanol synthesis reactions are reversible it is essential to remove excess heat to ensure sufficient conversion. There are 3 principally different reactors in which this can be achieved (figure 2).
In the tubular reactor (C) a desirable temperature profile is obtained, but this reactor type is mechanically complicated and therefore relatively expensive.
Quench cooling (B) leads to an undesirable temperature profile, so that a large volume of catalyst is required. The profile obtained with indirect cooling (A) is intermediate.


S1
S2
S3
R1
H1
H2
H3
H4
H5
H6
H7
C1
C2
C3
C4
C5
Co1
Co2
D1
D2
F1
T1
T2
P1
P2
water
steam
natural gas
oxygen
water
purge
light ends
methanol
ethanol
water
C cooler
Co compressor
D condensate drum
F flasher
H heat exchanger
R reformer
S synthesis reactor
T distillation tower
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G.H. v Heusden B. A. Snoodijk
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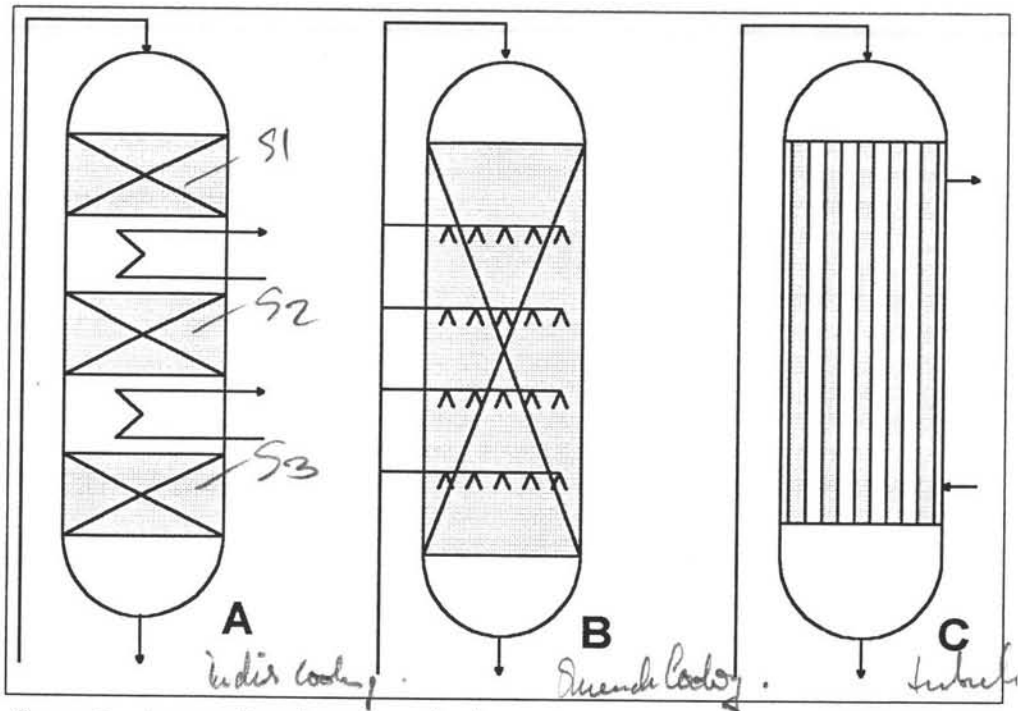


figure 2 types of methanol synthesis reactors

The advantages of indirect cooling over quench cooling are:
- higher conversion can be obtained since there is no dilution with unconverted quench gas
- reaction heat can be recovered for useful purposes
- first bed can act as guard for the remaining bed in case of any poison in the feed.

In this design is chosen for indirect cooling because in this way the reaction heat of the methanol synthesis can be used to heat the feeds of the reformer.

2.2 Proces flow diagram

After cleaning the natural gas feed is preheated by heat-exchanger H3 which is using the heat of the synthesis reaction. Then the gas is mixed with an excess of steam. To keep the amount of steam constant there is a small water feed present. This water plus the recycled water is vaporised and preheated by heat-exchangers H1. The steam natural gas flow is heated in heat exchangers H2 until 900 K. Both H1 and H2 use the reactor outlet to heat the flows.

In the reformer (R1) part of the natural gas is burned, the heat of this reaction is used for the endothermal reforming reaction. The reformer converts the methane and steam into synthesis gas ($CO+H_2$). The reactor outlet is cooled down by heating the feed of the reformer in heat-exchanger H1 and H2. Finally the flow is cooled down until 300 K. Then in condense drum (D1) the water is separated from the synthesis gas. The water is recycled.

The synthesis gas is compressed and preheated by the heat of the synthesis reactor in heat exchanger H5. The gas then is mixed in the recycle flow of the synthesis reactor. The gas then enters the synthesis reactor where it is converted in three beds into methanol. After each bed

the flow is cooled. The heat after the first bed is used to preheat the natural gas feed (H3), after the second bed the heat is used to heat up the recycle of the reactor itself and after the third bed the heat is used to preheat the feed of the synthesis reactor and to reboil the bottom flow distillation column T1. The gas is cooled down until 300 K and the methanol is separated from the unreacted synthesis gas in drum D2. The unreacted gas is recycled, part of it is drained.

The light by products of the methanol synthesis reaction and the reforming reaction are flashed out of the methanol in flash drum F1. The water is removed in distillation column T1 out of the methanol. Finally in column T2 the ethanol is removed out of the methanol.

Chapter 3 Equipment

3.1 The reactor designs

Both reactors are designed by first calculating the amount of catalyst needed. Then particle or rod dimensions are chosen. Pressure drops then determine the dimensions of the outer shell of the reactor.

3.1.1 Catalysts

The catalyst in the reformer is a nickel on alumina catalyst and in the synthesis reactors a Cu/ZnOxide on alumina catalyst is used.
The calculation of the amount of catalyst needed is a very complex mathematical problem. It boils down to very complex multidimensional differential equations that need to be solved. This can not be done analytically so computer software is required. A Pascal program is written which calculates concentration and temperature profiles.

3.1.2 General explanation for both reactors:

The total mass balance over the reactor is:

$$\text{out} = \text{in} - \text{conversion} \qquad (7)$$

$$C|_{x=L} = C|_{x=0} - \int_0^G (r(C,T,P))dx \qquad (8)$$

in which C is a vector of concentrations, all unknown functions of x,
T is temperature, also an unknown function of x,
P is pressure, responding to change of total amount of moles,
r represents an overall dC/dx, composed of one or more rates of reaction.
G is the total amount of catalyst needed.

Dividing the reactor in N slices (N being very large) one can assume every slice to be a homogenous mixture of catalyst and chemicals in which r is constant. A mass balance over a slice is:

$$C|_{x+\Delta x} = C|_x - r(C|_x, T|_x, P|_x) * \Delta x \qquad (9)$$

in which all variables are constants ($\Delta x = G/N$).

Calculating the entire tube slice by slice, each time taking output conditions of a preceding slice as input conditions of a next slice until a certain wanted conversion is reached, supplies the amount of catalyst needed.
The function r(C,T,P) is very complex. r is calculated via fugacities or partial pressures, all being dependent of Temperature, Pressure, compound characteristics, equilibrium constants, catalyst activities and composition.

An Enthalpy balance is used to calculate the temperature profile; H=0 over a slice as well as over the entire tube.

What actually takes place is:

$$T/_{x+x} = T/_{x} + (\ r_{i,x} * \ x * H_{r,i}(T,P))/Cp(T,C) \qquad (10)$$

so that: $H_{in}(T_1, C_{in}, P_1) = H_{out}(T_2, C_{out}, P_2)$ (11)

This equation is simultaneously solved during the slice by slice calculation of the concentration profiles. This is done by calculating the temperature at x+x (T_2) at which the enthalpy of the slice leaving stream is the same as the enthalpy of the slice entering stream. These calculations have to be simultaneously because all equilibrium, reaction rates and activities involved are strongly dependant of temperature.

The way vector C changes with r follows directly from the reactions that occur. Should there be just one reaction, the whole of vector C could be written in one variable, for instance a conversion variable. When more reactions occur this is not possible.

Pressure changes due to conversion proved to be of very little influence on the amount of catalyst needed and are therefor left out of consideration.
The total of complexity and extensiveness of the above made it impossible to use the standard mathematical software like RRstiff or Psi/C. Therefor a Pascal program was developed, which calculated all profiles in the reactors.

Iterative procedures are all done by the most simple half value method; the differential equations are all solved with the fourth order Runge Kutta method.

3.1.2.1 The reformer

The kinetics in the reformer concern only one reaction:

$$CH_4 + H_2O \text{ --> } CO + 2H_2 \qquad (1)$$

A very simple model was found:

$$-dCH_4/dt = r = k * P_{CH4} \text{ [mol/min g cat]} \qquad (12)$$

in which r = rate of reaction [mol/min g_{cat}]
k = reactionconstant [mol/min g_{cat} atm]

k is temperature dependant

$$k = A * \exp(-B/T) \qquad (13)$$

in which A = 5.95097e7 [mol/min g_{cat} atm]
B = 20960.4 [K]

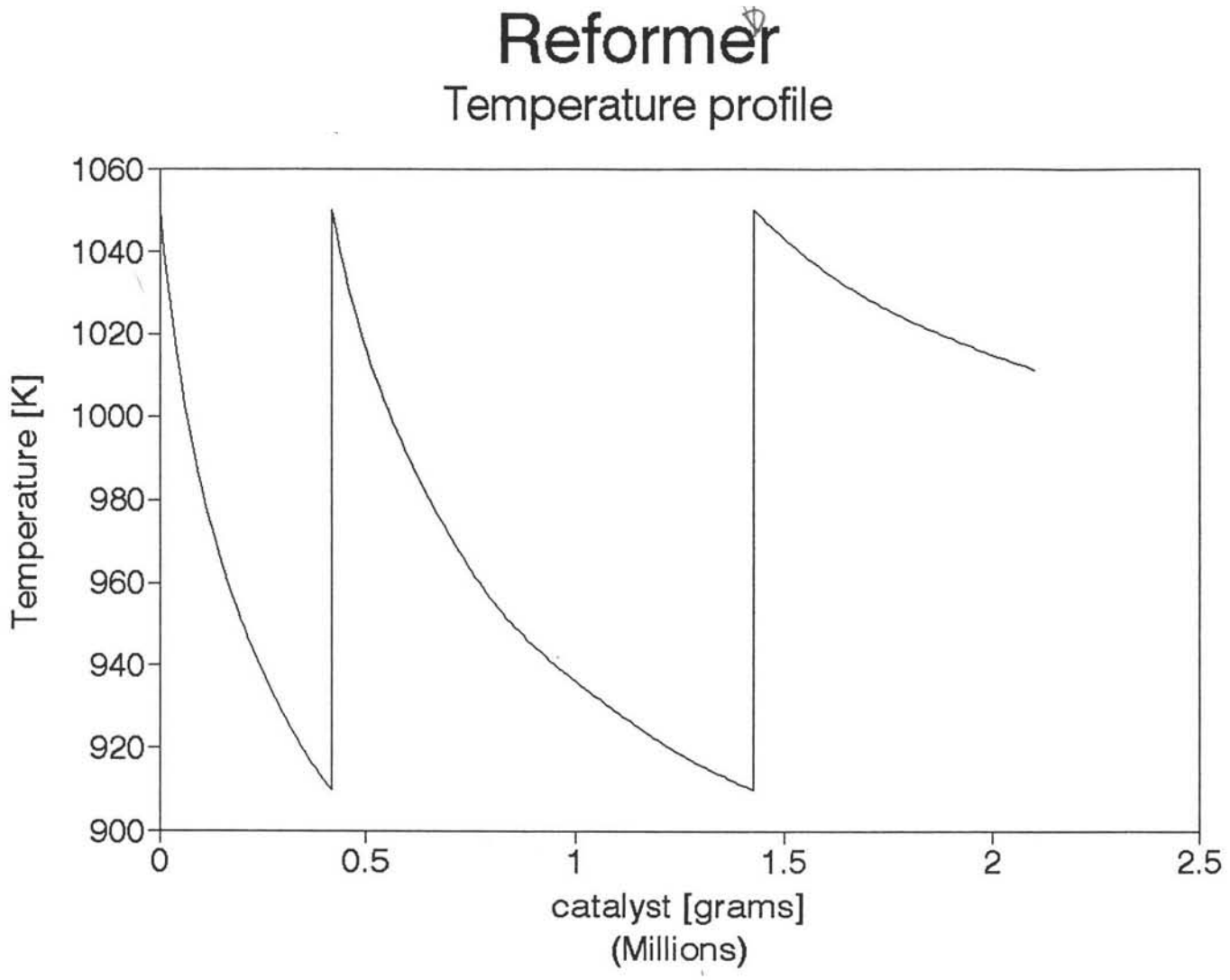


figure 3 temperature profile of the reformer

These values were determined by Agnelli et al. [12] by measurements on a reactor with very fine grinded catalyst and a very small flow. Therefore no diffusion limitation was taken into account.
In this reformer a larger catalyst is used so diffusion limitations have to be taken in consideration. To model the reactor a porous slab tube model is used.
A variable efficiency (E) was calculated in each step of the integration.

hence: $-dCH_4/dt = r = E*k*P_{CH4}$ [mol/min g_{cat}] (14)

The calculation of E is explaind in appendix E.

The temperature profile was calculated as explained in 3.1.2. When while calculating through the tube the temperature became too low, an oxygen injection takes place, which is visible in figure 3; the methane concentration clearly drops very steep. As much methane is (partially) burned here as needed to bring the temperature of the flow to its original height.
The concentration profiles is shown in figure 4.

The calculated amount of catalyst for the reformer is 2200 kg.

3.1.2.2 The synthesis reactor

Methanol is formed from both CO (4) as from CO_2 (6). Besides these two methanol forming reactions the water-gas shift reaction (2) also has to be taken into account.
From equations 4 and 6 follows that the methanol formation is favoured by decreasing temperature and increasing pressure. The reactions rates will increases with higher temperature and decreases with a higher conversion to methanol.

To insure a high reaction rate and a reasonable conversion the temperature is chosen between 500 and 600 K.
A high pressure will result in costly material specification, therefor is chosen to operate the methanol synthesis with medium pressure (100 bar).

For the design of the methanol synthesis reactor, the kinetic results reported by Takagawa and Ohsugi [1] have been used to simulate the reaction rates for the methanol synthesis from CO, CO_2 and H_2 over a copper-zinc based catalyst:

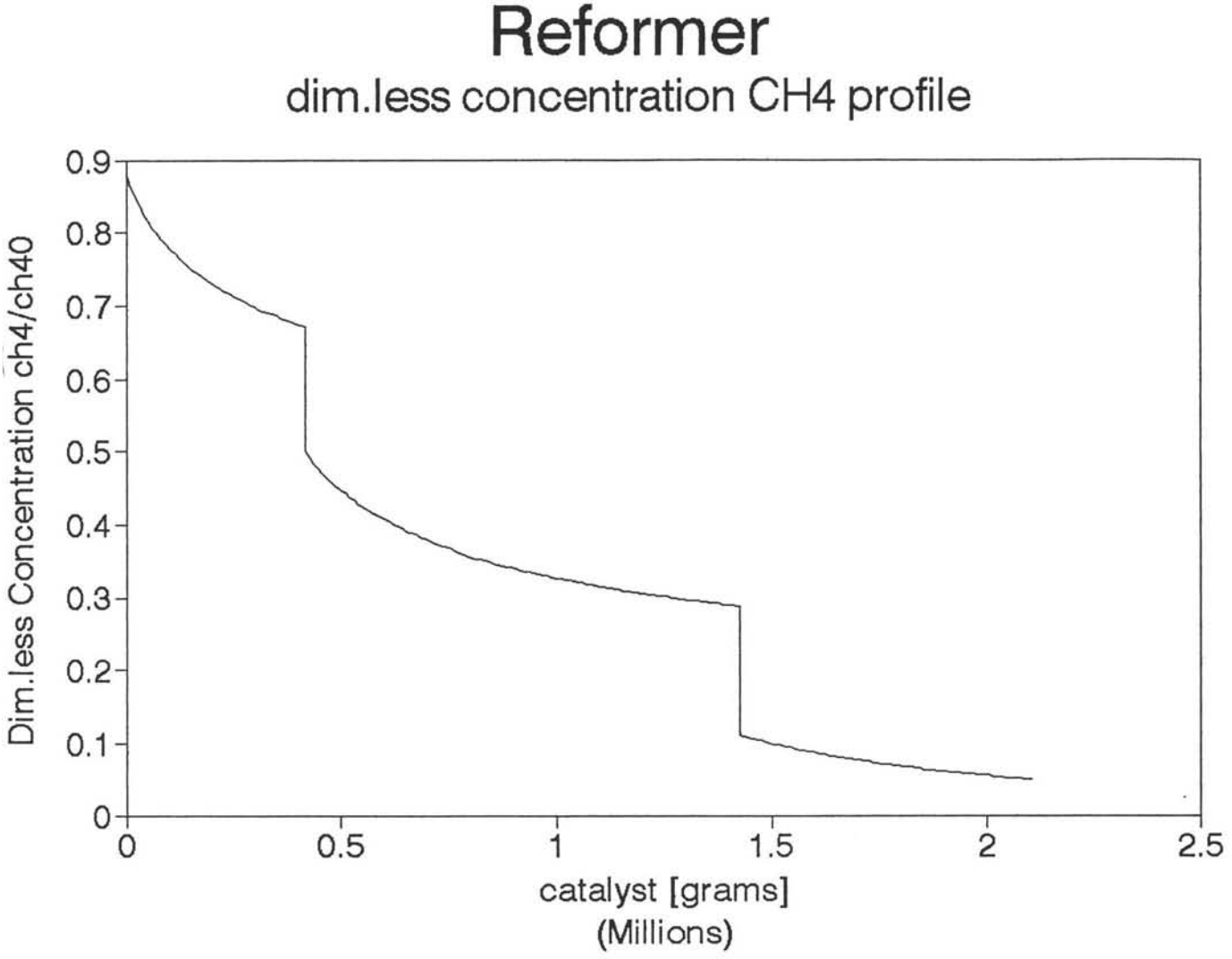


figure 4 concentration profile of the reformer

$$r_1 = \frac{k_1 \cdot \left(f_{CO} \cdot f_{H_2}^{a1}\right)^{a2} \cdot \left\{1 - \left(\frac{f_{CH_3OH}}{K_1 \cdot f_{CO} \cdot f_{H_2}^{2}}\right)^{b}\right\}}{1 + K_{CO_2} \cdot f_{CO_2} + K_{H_2O} \cdot f_{H_2O}} \qquad (15)$$

$$r_2 = k_2 \cdot f_{H_2} \cdot \left(1 - \frac{f_{CO} \cdot f_{H_2O}}{K_2 \cdot f_{CO_2} \cdot f_{H_2}}\right) \qquad (16)$$

$$r_3 = \frac{k_3 \cdot f_{CO_2} \cdot \left(1 - \frac{f_{CH_3OH} \cdot f_{H_2O}}{K_3 \cdot f_{CO_2} \cdot f_{H_2}^{3}}\right)}{1 + K_{H_2O} \cdot f_{H_2O}} \qquad (17)$$

where r_i is the rate of reaction i (equation 1- 3) in moles per litre catalyst hour , k_i the rate constant of reaction i and f_i the fugacity of component i in atm.
K_{CO2} and K_{H2O} are the adsorption equilibrium constants of CO_2 and H_2O, respectively;
a_1, a_2 and b are constants. The parameter estimates are shown in table 2, where the temperature is in Kelvin and R is 1.987 cal/mol K :

Table 2 Parameter Estimates of the Rate Expressions:

$a_1 = 2.5,\ a_2 = 0.35,\ b = 0.8$
$k_1 = 1.03\text{x}10^{7}\ \exp(-16.6\text{x}10^{3}/R*T)$
$k_2 = 1.25\text{x}10^{12}\ \exp(-28.8\text{x}10^{3}/R*T)$
$k_3 = 2.33\text{x}10^{7}\ \exp(-15.0\text{x}10^{3}/R*T)$
$K_{CO2} = 1.86\text{x}10^{-9}\ \exp(18.1\text{x}10^{3}/R*T)$
$K_{H2O} = 1.06\text{x}10^{-7}\ \exp(16.7\text{x}10^{3}/R*T)$

The fugacity of the components are calculated according to the Soave-Redlich-Kwong (SRK) Equation of State .

The equilibrium constants were obtained as function of temperature from Klier et al. [2] :

$$K_1 = \frac{3.27\text{x}10^{-13} \cdot \exp(11678/T)}{1 - (1.95\text{x}10^{-4} \cdot \exp(1703/T) \cdot p)} \qquad (18)$$

$$K_3 = \frac{3.826 \cdot 10^{-11} \cdot \exp(6851/T)}{(1 - (1.95 \cdot 10^{-4} \cdot \exp(1703/T) \cdot p)) \cdot (1 - (4.24 \cdot 10^{-4} \cdot \exp(1107/T) \cdot p))} \qquad (19)$$

$$K_2 = \frac{K_3}{K_1} \qquad (20)$$

where T is in Kelvin and p in atm.

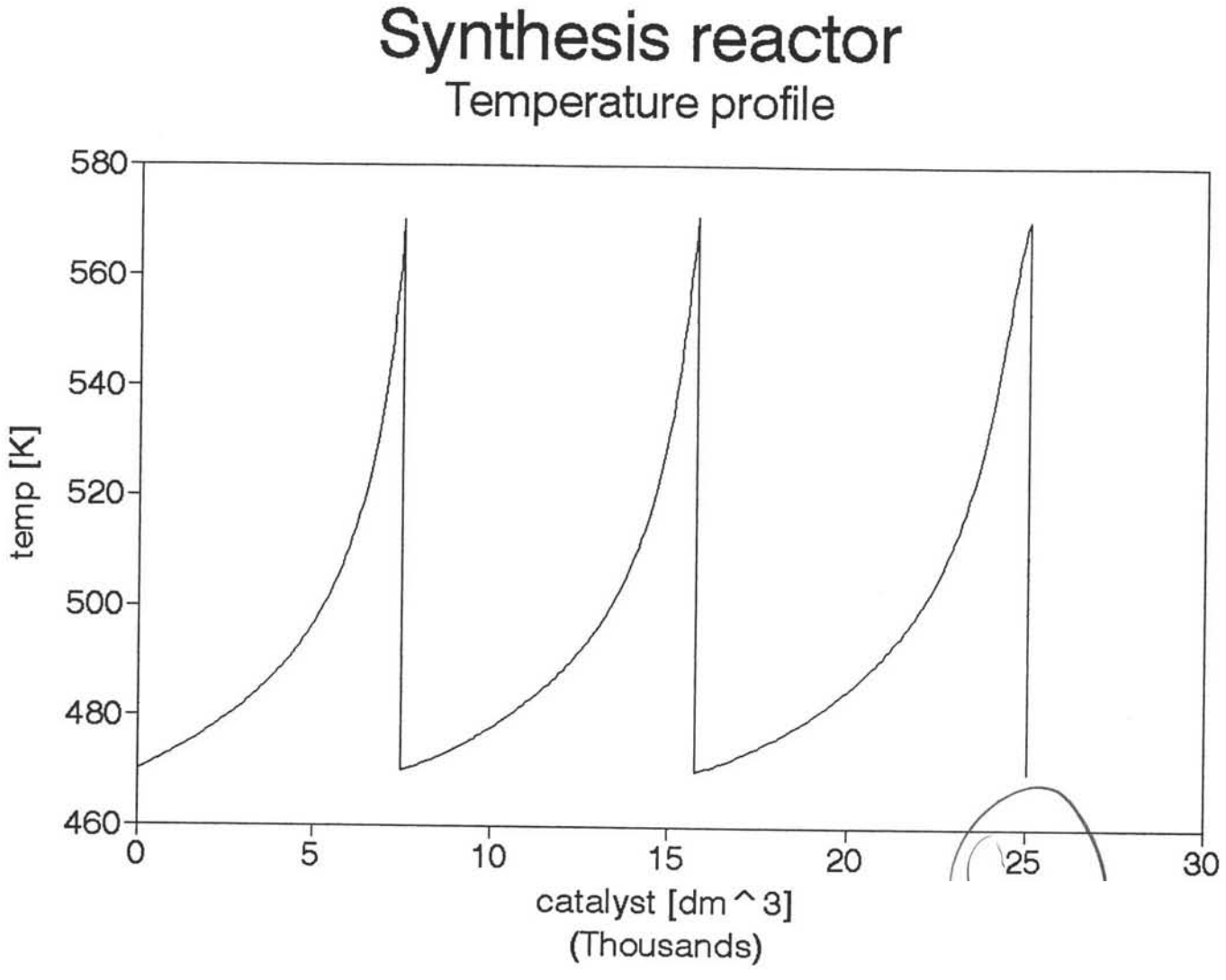


figure 5 temperature profile of the synthesis reactor

The equations to calculate the reaction rates and the equilibrium constants were selected because they were obtained under the same conditions as are chosen for this design of the methanol synthesis.

Here also the temperature profile is calculated as described in 3.1.2. (figure 5). When temperature became too high, the calculation simply dropped it to its original value.
The concentration profile is shown in figure 6.

The calculated amount of catalyst needed for the synthesis reactor is 25 m^3

3.1.2.3 Reformer dimensions

Chosen is a rod diameter (D_0) of 5 mm. The diameter of the rod core without catalyst layer (D_1) is 4 mm. Pitch is set as $1.2*D_0$;
The total number of rods is :

$$N = G/(\rho_c L * \pi * (D_0^2 - D_1^2)) \qquad (21)$$

In which
- G : amount of catalyst in kg
- ρ_c : density of catalyst in kg/m^3
- L : length of the rods in m

A pressure drop of 10% otal pressure is preferable and L can now be calculated by:

$$p/L = 4*f*(1/D_h)*1/2*\rho*v_{gem}^2 \qquad (22)$$

in which
- p/L : the pressure drop per meter in Pa/m
- f : the friction factor of the rod bundle
- v_{gem} : is the superficial velocity in m/s
- ρ : is the density of the gasmixture in kg/m^3
- D_h : hydraulic diameter in m

$$D_h = (D^2 - N*D_0^2) / (D + N*D_0) \qquad (23)$$

in which
- D : Reactor diameter in m

$$v_{gem} = \phi/A$$

in which
- ϕ : flow in m^3/s
- A : front surface in m^2

$$A = 0.25*\pi*D^2 \qquad (24)$$

A can be calculated with N ; for a regular triangular array the formula is:

$$A = 4*N*S^2*0.5*\sqrt{3} \qquad (25)$$

in which
- S : pitch in m

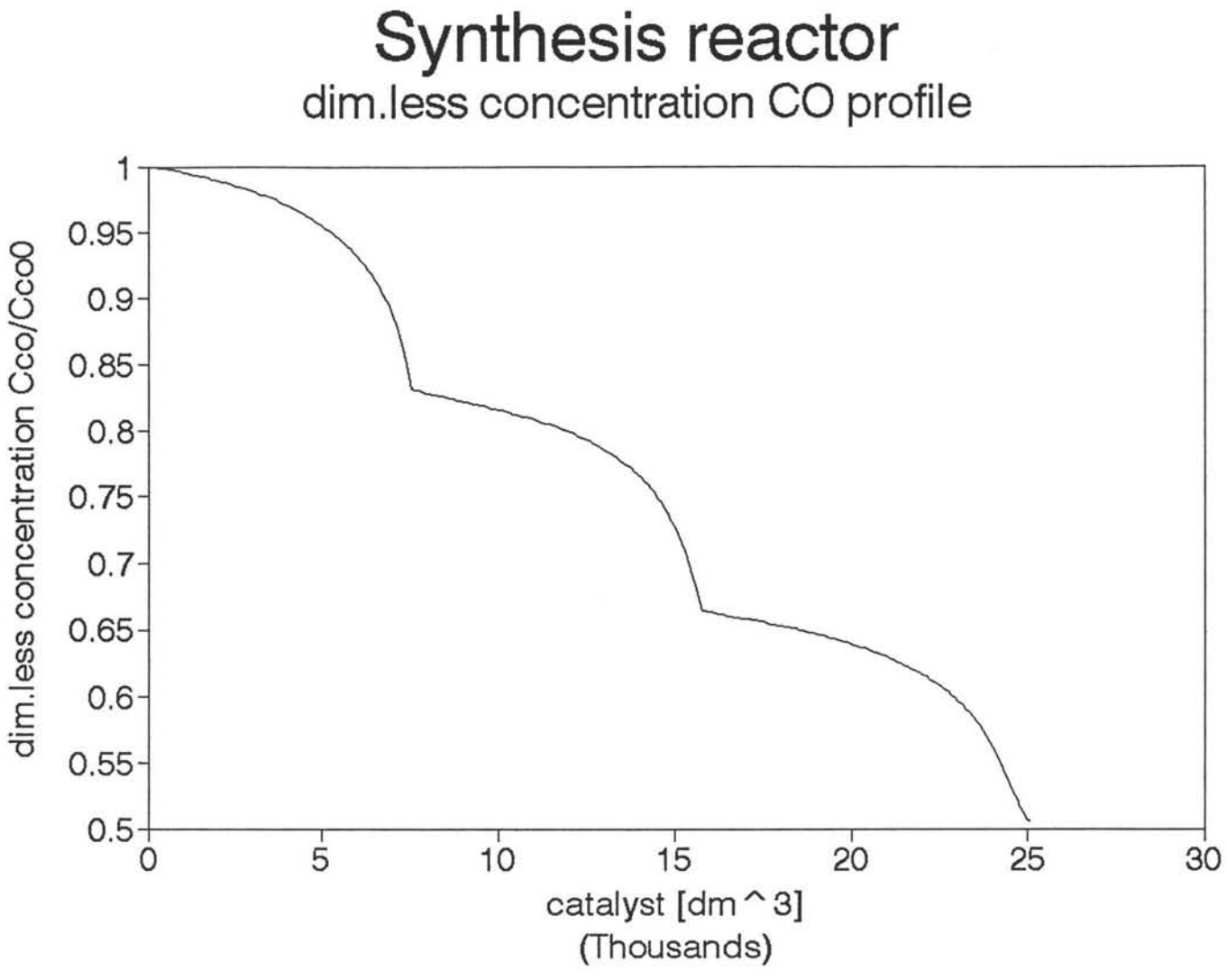


figure 6 concentration profile of the synthesis reactor

$$S = Mw*P_{tot}/(R*T) \qquad (26)$$

in which	Mw	:	mean molecular weight of the gas in kg/mol
	P_{tot}	:	total pressure in Pa
	R	:	gas constant in J/molK
	T	:	temperature in K

f is calculated by

$$4*f = (0.57+0.18*(S/D_0 1)+0.53*(1\exp(a)))*4*ftube \qquad (27)$$

$$a = 0.58+9.2*(S/D_0 1) \qquad (28)$$

$$1/ftube = (3.481.7372*\ln(2*h/D_h+9.35/(Re*ftube^{0.5})))^2 \qquad (29)$$

in which	ftube	:	friction factor in a normal tube
	h	:	roughness in m
	Re	:	reynolds number in a tube

$$Re = \rho *v_{gem}*D_h/\eta \qquad (30)$$

in which η : mean viscosity of the gas in Pa s

further constants needed for the calculation are:

ρ_c	= 1020	[kg/m^3]
ρ	= 2.887	[kg/m^3]
h	= 1e-5	[m]
ϕ	= 27.10	[m^3/s]
η	= 3.5e-5	[Pas]
T	= 1000	[K]
P	= 10e5	[Pa]
R	= 8.3144	[J/molK]
G	= 2200	[m^3]

The above set of equations is solvable with MERCURY if either N or L is chosen.
After much concideration we chose N to be 88,000 rods. This resulted in a tank with the following dimensions:

Reformer:

length	: L	=	6.57	[m]
diameter	: D	=	1.87	[m]
number of rods	: N	=	88,000	[-]
bed porosity	: ε	=	0.37	[-]
pressure drop	: P	=	0.98e5	[Pa]

3.1.2.4 Synthesis reactor dimensions.

The amount of catalyst needed was 25 m^3. The reactor is made of three reactors with in between a heat exchanger. Figure 5 and 6 show how much catalyst is put in each tank.

reactor 1: 7.5 [m^3 cat]
reactor 2: 8.0 [m^3 cat]
reactor 3: 9.5 [m^3 cat]

The corresponding volumes are those of the catalyst volume divided by the bed porosity of 0.4 , given by Lee et al. [3] :

reactor 1: 12.5 [m^3]
reactor 2: 13.3 [m^3]
reactor 3: 15.8 [m^3]

Taking in regard a L/D- ratio of about 2 and a general diameter of 3 [m] follows:

reactor 1: L=5.6 D=3
reactor 2: L=5.9 D=3
reactor 3: L=7.0 D=3

3.1.2.5 wall thickness

The formula to estimate the wall thickness (in m) of a reactor with internal pressure is (in British standard (BS5500)):

$$e=P_i D_i/(4f-1.2*P_i) \qquad (31)$$

in which P_i : internal pressure in Pa
D_i : internal diameter in m
f : design stress in Pa

The used material is stainless steel;
the design stresses of stainless steel are:

T = 1000K : f = 90 [N/mm^2]
T = 500K : f = 110 [N/mm^2]

The wall thickness of the reformer is calculated to be:

10e5*1.8/(4*90e6-1.2*10e5) = 5e-3 m = 5 mm.

A practical thickness is 7 mm, which insures sufficient rigid to withstand its own weight, and any incidental loads for any vessel.

The wall thickness of the three synthesis reactors are:

100e5*3/(4*110e6-1.2*100e5) = 70 mm

3.2 Other equipment

The specification of the equipment can be found in appendix D, a list of equipment is given in appendix C.

3.2.1 Heat exchangers.

All heat exchangers have shells and pipes of stainless steel with a chromium content above 12 per cent. A chromium alloy is chosen because of it's good resistance against high temperature corrosion. Stainless steal also resists the high pressures and temperatures. All tubes are 20 mm outside diameter and 5 m long.

The shell thickness of the heat exchangers is estimated using equation 31.

The overall heat-transfer coefficients are estimated, CHEMCAD III is used to calculate the tube surfaces. The pressure drop is assumed to be zero.

Heat exchanger 1

H1 contains one heat exchanger which preheats the water, it operates at 10 bar. It has:

Number of tubes	:	3114
Shell diameter	:	1.5 m
Wall thickness	:	8.3 mm (calculated)
		12 mm (real)

H1 also contains eight heat exchangers in series which used to vaporise the water, they operate at 10 bar. They each have:

Number of tubes	:	2874
Shell diameter	:	1.5 m
Wall thickness	:	8.3 mm (calculated)
		12 mm (real)

Heat-exchanger 2

H2 heats the reformer feed up to 900 K, it contains five exchangers in series. H2 operates at 10 bar, they each have:

Number of tubes	:	2799
Shell diameter	:	1.5 m
Wall thickness	:	8.3 mm (calculated)
		12 mm (real)

Heat-exchanger 3

H3 heats the natural gas feed using the heat of the synthesis reaction, the shell side operates at 100 bar, the tube side operates at 10 bar. It has:

Number of tubes	:	2975
Shell diameter	:	1.5 m
Wall thickness	:	60 mm (calculated)
		70 mm (real)

Heat-exchanger 4

H4 heats up the recycle flow of the synthesis reactor, it uses the heat of the synthesis reaction. It operates at 100 bar and has:

Number of tubes	:	2920
Shell diameter	:	1.5 m
Wall thickness	:	60 mm (calculated)
		70 mm (real)

Heat-exchanger 5

H5 heats up the synthesis reactor feed, it also uses heat of the synthesis reactor and also operates at 100 bar. It has:

Number of tubes	:	2277
Shell diameter	:	1.5 m
Wall thickness	:	60 mm (calculated)
		70 mm (real)

3.2.2 Coolers.

The coolers operate at lower temperatures then the heat exchangers, therefore there is no need for using chromium alloys. Because the cooling water can be corrosive and erosive the tubes are made of cupro-nickel alloys. Cupro-nickel have very good resistance to corrosion-erosion. The tube size is again; 20 mm outside diameter, 5 m length. The shells are made of stainless steel.

The overall heat transfer coefficient of the coolers is estimated, CHEMCAD III is used to calculate the tube surfaces. The pressure drop is assumed to be zero.

The wall thickness is calculated in the same way as was done for the heat exchangers.

Cooler 1.

C1 cools down the water synthesis solution to 300 K, and operates at 10 bar. River water is used as coolant. It has:

Number of tubes	:	2000
Shell diameter	:	1.3 m
Wall thickness	:	7.2 mm (calculated)
		10 mm (real)

Cooler 2.

C2 cools down, in between two beds of the synthesis reactor, until 470 K. It operates at 100 bar. River water is used as coolant, C2 has:

Number of tubes	:	111
Shell diameter	:	0.4 m
Wall thickness	:	16 mm (calculated)
		20 mm (real)

Cooler 3.

C3 cools the methanol/synthesis after the reactor solution down until 300 K. It operates at 100 bar and river water is used as coolant. It has:

Number of tubes	:	1380
Shell diameter	:	1.2 m
Wall thickness	:	49 mm (calculated)
		60 mm (real)

3.2.3 Distillation columns.

The plate spacing of the distillation columns is chosen to be 0.5 meter. The diameter of the column can be calculated using the following formulas.

$$u_v = (-0.171 \cdot l_t^2 + 0.27 \cdot l_t - 0.047) \cdot \left[\frac{\rho_l - \rho_v}{\rho_v} \right]^{0.5} \qquad (3$$

Where l_t (m) is the plate spacing and $\hat{u}_v$ (m/s) the maximum vapour velocity.

The column diameter is then calculated using:

$$D_c = \sqrt{\left(\frac{4 \cdot V_w}{\pi \cdot \rho_v \cdot u_v}\right)} \qquad (33)$$

V_w is the maximum vapour flow (m^3/s), D_c is an estimation for the column diameter (in m).

The wall thickness can be calculated using formula 31??. It has to be considered that the towers also have to with stand the forces of the wind.

The number of plates is calculated using the shortcut procedure of CHEMCAD III.

Tower 1

Column T1 is used to remove the water from the methanol, 99 per cent of the methanol has to flow over the top, 1 per cent of the water is allowed to flow over the top. It has:

Number of plates	:	28
Plate distance	:	0.5 m
Height	:	15 m
Diameter	:	0.95 m
Wall thickness	:	25 mm (real, because of the height of the tower)

Tower 2

The distillation column T2 is used to remove the ethanol from the methanol. Again 99 per cent of the methanol flows over the top and 1 per cent of the ethanol is allowed to flow over the top.

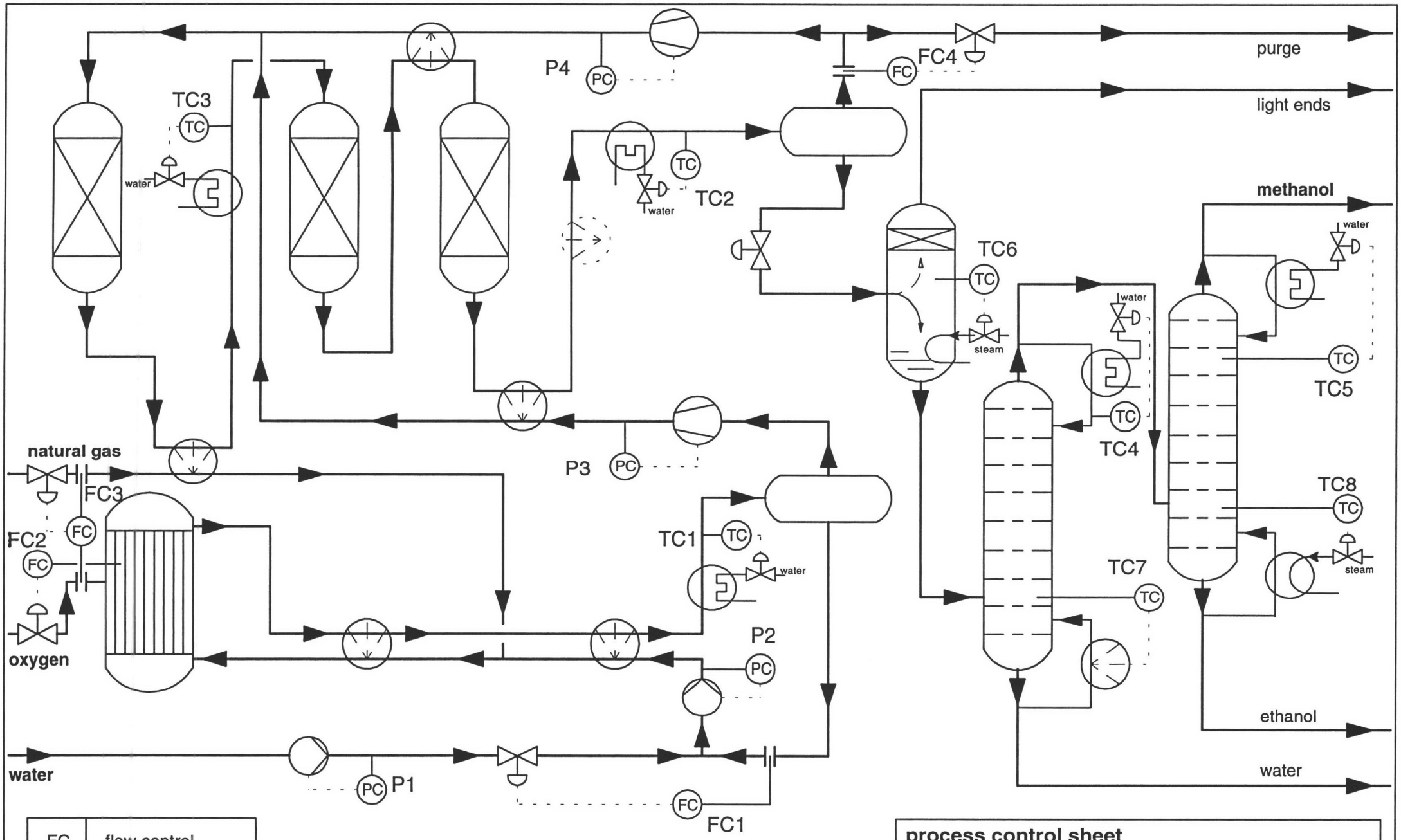
Number of plates	:	35
Plate distance	:	0.5 m
Height	:	18.5 m
Diameter	:	2.0 m
Wall thickness	:	30 mm (real, because of the height of the tower)

3.2.4 Flash drum.

The flash drum is made of stainless steel. The heating tubes are made of stainless steal with a minimum of twelve per cent of chromium. The steam can cause corrosion.

3.2.5 Pumps and compressors

All pump are centrifugal pumps which need to pump no corrosive liquids. Compressor Co2 is a normal compressor, Co1 is a mufti stage intermediate cooled compressor. There are four compressor stages and three coolers. The coolers cool down from 380 K to 300 K.



FC	flow control
P	pressure control
TC	temperature control

process control sheet
methanolsynthesis

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Chapter 4 Process control

4.1 Flow control

Flow Control 1.

FC 1 controls the water feed of the system. Extra water has to be adjusted because not all of the water is condensated in the condensate drum (d1). The controller measures the water flow out of the condensate drum (d1) and compares the measured flow with the set point of the water flow in the reformer (r1). The difference between the two flows is added. This is an feedforward type of flow control.

Flow Control 2

FC 2 controls the oxygen feed of the reformer (r1). The temperature of the flow out of the reformer (r1) is measured. This temperature is compared with the set point. When the temperature is lower then the set point extra oxygen is added, when the temperature is higher then the set point less oxygen is added. This control also serves as an safety. When the temperature reaches an alarm value the oxygen flow is closed. This is an feedback flow control system.

Flow Control 3

FC 3 controls the natural gas feed of the reformer (r1). The needed natural gas feed depends on the oxygen feed into the reformer (r1). Therefore the natural gas feed is controlled by measuring the oxygen feed (after the oxygen feed controller FC 2). The natural gas feed is a set proportion of the oxygen feed. As an alarm temperature is reached in the reformer (r1) the oxygen flow becomes zero and therefore also the natural gas flow becomes zero. The natural gas feed controller is a feedforward flow control system.

Flow Control 4

FC 4 controls the amount of gas which is drained in the recycle loop of the synthesis reactor (s1 to s3). The drain is very important, it avoids accumulation of pollution in the synthesis reactor (s1 to s3). The drained amount of gas is a ratio of the flow out of the condensate drum (d2). Therefore the flow out of the condensate drum (d2) is measured. The set ratio of the gas flow is drained. This is a feedforward flow control system.

4.2 Pressure control

Pressure Control 1

PC 1 controles the pressure of the water feed. The water enters the plant at 7 bar, it has to be 10 bar. The pressure is measured after the water feed pump (p1), if needed the power of the pump is adjusted. This is a feedback pressure control system.

Pressure Control 2

PC 2 controls the pressure of the water feed of the reformer (r1). It measures the pressure before the pump (P2) and adjust if necessary the input power. This is a feedforward control system.

Pressure Control 3

PC 3 controls the compressor system (Co1) which increases the pressure from 10 to 100 bar which is the pressure needed in the synthesis reactor (s1 to s3). The control system measures the pressure only after the last compressor. This is the only compressor with an adjustable power, the other compressor (of system Co1) compress maximum.
This is also a feedback pressure control system.

Pressure Control 4

PC 4 controls the pressure of the reflux flow of the synthesis reactor (s1 to s3). Because of the pressure drops of the packed beds of the reactor the pressure of the reflux flow is less the 100 bar. Therefore the pressure has to be increased by a compressor (Co2). The pressure after the compressor is measured, if needed the power of the compressor is adjusted.

4.3 Temperature control

4.3.1 Coolers

Temperature Control 1 and Temperature Control 2

TC 1 and TC 2 control the temperature of the feed flows of the condensate drums (d1 and d2). The flows need to be cooled down so enough of the water respectively methanol is condensated. The temperature after the coolers is measured, if needed the flow of coolant is adjusted. These are feedback temperature control systems.

Temperature Control 3

TC 3 cools down the flow in the synthesis reactor between the first two beds (s1 and s2). The temperature is measured after the cooler, if needed the flow of the coolant is adjusted. This is a feedback temperature control system.

(Temperature Control 4) and Temperature Control 5

TC 4 and TC 5 control the condensation of the top flow of the two distillation towers (T1 and T2). The controller measures the top temperature of the column, if needed the flow of the coolant is adjusted. These are feedback control systems.

4.3.2 Heaters

Temperature Control 6

TC 6 controls the temperature in the flash drum (f1). The temperature must be high enough to flash most of the dimethylether. The temperature is measured in the gas phase, if needed the steam flow in the heater is adjusted. This is a feedback temperature control system.

(Temperature Control 7) and Temperature Control 8

TC 7 and TC 8 control the reboiling of the bottom of the distillation towers (T1 and T2). The temperature of the bottom of the column is measured, if needed the steam flow in the heater is adjusted. This is a feedback temperature control system.

Chapter 5 Safety

All human behaviour can cause all sorts of hazards and risks, so it can cause certain damage or losses. Safety is a condition in which these hazards and risks are very small, there is very little chance something is damaged.
The methanol process must of course be operated safely. Prevention of hazards and risks is the first step. Therefore:

- the prescriptions of the permit should be observed,
- the hardware, like instrumentation and safety equipment, should be controlled often,
- the operators should well trained,
- instruction for process control,
- fire proof clothes,
- well trained fire brigade,
- good and well known escape routes,
- a contingency plan should be available and well known by the employees,
- good communication equipment should be available,
- good maintenance.

Also the equipment must be safe and safe to operate. Therefor we now take a closer look at the two most dangerous equipment's of the process, the reformer and the synthesis reactor.

The reformer

In the reformer pure oxygen is introduced which is burned instantly. Therefore no explosive gas can be formed. When more oxygen enters the reformer or when less methane enters the reformer there still will be a surplus of methane so still no explosive gas can be formed. When too much oxygen is introduced the temperature can become to high, therefore a high temperature alarm should be connected with the oxygen flow control. Only when no methane enters the reactor oxygen can flow to the synthesis reactor where it can react with the hydrogen a runaway can take place. Therefore a low flow alarm is installed on the methane flow (see chapter beschrijving flow schema plus alarm).
Because an endothermic reaction occurs in the reformer the chance that a runaway will take place in the reformer is very little.In table 3 a HAZOP for the reformer is given.

table 3 HAZOP for the reformer:

No, not	No flow of: - methane - steam - oxygen	- No reforming, the oxygen flows to the synthesis reactor. Low flow alarm should be installed. Risk. - No reforming, temperature rises, low flow alarm should be installed. Risk. - Reformer cools down, reforming stops, low flow alarm should be installed.
More	More flow of: - methane - steam - oxygen More pressure More temperature	- No stoechiometric reforming. Flow control should be installed. - Loss of energy. - Temperature rises, temperature alarm should be connected with oxygen flow control. Risk. - The equilibrium goes to the wrong side. - Equilibrium goes to the good side. The temperature must not rise to much.
Less	Less flow of : - methane - steam - oxygen Less pressure Less temperature	- No stoechiometric reforming. - Less excess of steam, reforming almost normal. - No stoechiometric reforming. - Equilibrium goes to the good side. - Equilibrium goes to the wrong side.

The synthesis reactor

The risk of a run away in the synthesis react is given by the following formula:

$$\varepsilon = \frac{E}{R \cdot T_r^2} \cdot \frac{\Delta T_{ad}}{(1 + \frac{\Delta T_{ad}}{T_r})} \qquad (34)$$

Where: Tr : is the reaction temperature
Tad : is the maximum reachable adiabatic temperature
E : the activation energy
R : the gas constant

When $\varepsilon < 10$ there is little risk for a run away, $\varepsilon = 6.8$ so the synthesis reactor has no risk for a runaway.
The material off the synthesis reactor must be able to stand the high pressures which occur during normal operation. The operators should be aware of the dangers of the high pressure.
A HAZOP for the synthesis reactor is given in table 4 .

table 4 HAZOP for the synthesis reactor:

No, not	No flow of: - hydrogen - CO	 - No reaction, CO in distillation towers. - No reaction, hydrogen in distillation towers.
More	More flow of: - hydrogen - CO More pressure More temperature	 - Hydrogen in distillation towers. - CO in distillation towers. - Reaction rate goes up, change for a run away increases, pressure control should be installed. Risk. - More CO2 in stead of methanol.
Less	Less flow of : - hydrogen - CO Less pressure Less temperature	 - Less methanol. - Less methanol. - Reaction rate goes to zero. - Reaction rate goes to zero.

Health

Because non of the used chemical components are toxic or lethal there is no direct danger for the employees. Still a nurse should always be present to treat small injuries. When a disaster takes place there must be back up from a medical staff.
Because no toxic elements are used there is a small risk for the people living in the area.

Environment

The methanol process is a clean process. The only pollution is air pollution, small amounts of CO and CO2 will be present in the exhaust gas. The emissions should be kept very low.

Chapter 6 Economics

6.1 Introduction

In this chapter an economic evaluation is made of this design.
For making this evaluation some assumptions are made:

-the depreciation of this process is ten years and it has no salvage value
-taxes are 50%
-there is no borrowed capital

6.2 Investment costs

Two methods for determining the investment costs of this design are applied.

6.2.1 Scale-up method

In the literature [4] two investment costs for a methanol plant are found:
-production of 800 kton/y has investment costs of fl 200 million
-production of 100 kton/y has investment costs of fl 50 million

The investment costs of this design can now be calculated by using a scale-up relationship

$$C2/C1=(S2/S1)^R \qquad (35)$$

Here C1 and C2 are the costs and S1 and S2 the corresponding capacities.
The R value can be found in the literature [5,6] and for a methanol plant the value is +/- 0.6.
Calculating the investment costs by using the two known investment costs gives fl 122 million and fl 106 million respectively. The average value of $I_{Scale\text{-}up}$ = fl 114 million.

6.2.2 Taylors method

A more detailed method for calculating the investment costs is Taylors method.
The total investment cost I_{Taylor} is calculated with:

$$I_{Taylor}=93*1000*f*P^{0.39}*C_I/300 \qquad (36)$$

in which f is the costliness index
P is the capacity in kT/y
C_I is index of EPE (=310 in june 1978)

The investment is found in dollars.
In this method process steps get scores for complexity. This total score is transformed into the costliness index f by a relating table.
In the next figures is the calculation of the costliness index for this design is found

Storage	Throuhput	M of C	Pressure/ Temperature	Total Score	Costliness Index
natural gas	-0.7	0	0	-0.7	0.9
oxygen	-0.7	0	0	-0.7	0.9
water recycle	2.6	0	0	2.6	2.0
synthesis gas	0.4	0	0	0.4	1.1
recycle syngas	1.3	0	0	1.3	1.4
methanol	0	0	0	0	1
Process					
reformer	3.2	1	1.3	5.5	4.3
seperator1	3.2	1	0	3.2	2.3
synthesis	2.3	1	2.3	5.6	4.4
seperator2	2.3	1	2.3	5.6	4.4
flasher	0.4	1	0	1.4	1.2
distillation1	0.2	1	0	1.2	1.1
distillation2	0.1	1	0	1.1	1.0
heat exch feed	3.2	1	2	6.2	4.9

					30.9

For P is 350 kTon/y this gives I_{Taylor}=$ 29.1 million. This value is multiplied by fl 2.34 /$, this factor contains location and exchange rate for 1978. Hence its divided by 115 and multiplied by 165 ,the costindexes of 1978 and 1994 with 165 estimated for 1994. This gives I_{Taylor}= fl 98.0 million.

This is lower than estimated with the scale-up method, a difference of 14%. It seems that both are 'rough' methods.

The total amount of catalyst is equal to 2200 kg (reformer) + 30.000 (synthesis reactor) = 32200 kg. The price of a catalyst is about 15/kg. The lifetime of the catalysts is estimated on 2 years. So the total money spend on the catalysts in ten years is about fl 2.4 million. This is hidden in the investment costs.

For further calculations I_t= fl 100.0 million will be chosen.

6.3 Operating costs

The operating costs K_f consists of the product volume dependant costs K_p, the maintenance and operating labour costs K_l and the investment dependant costs K_i. The cost of Sales, Administration and Research (SAR) is about 5% of the operating costs and so the total cost for a year K_t=1.05*K_f with K_f=K_p+K_l+K_i.

6.3.1 Product volume dependant costs

-natural gas,	$2.60*10^8$kg/y*fl 0.3095/kg	= fl 80.4 million
-oxygen,	$2.56*10^5$ton/y*fl 70/ton	= fl 17.9 million
-process water	$3.02*10^6$kg/y*fl 1.497/kg	= fl 4.5 million
-electricity	$1.51*10^8$kWh*fl 0.13/kWh	= fl 19.6 million
-cooling water	$3.07*10^7$m^3/y*fl 0.10/m^3	= fl 3.1 million

	Kp	= fl 125.5 million

6.3.2 Maintenance and operating labour costs

The operating costs are calculated with Wessels relation:

manhours/tons of product=k*N/(capacity/day) (37)

The factor k=1.07 for a continuous process in 1994 (corrected for increasing productivity of 6 % per year and k = 1.7 in 1986)
N is the number of process steps.
The following relationship can be derived from Wessels relation:

$L=20.3*N*C^{0.24}$ (38)

with L = total operating costs in k
N = number of process steps
C = capacity in kT/y

This is for a continuous process in 1994 for 350 k fl /functionplace.
For C=350 kT and N=3 (reformer, synthesis reactors, distillation towers)
this relation gives L=248 k .
Maintenance costs are estimated on 4% of the investment costs. This will be fl 4 million per year.
So K_l = fl 4.2 million

6.3.3 Investment dependant costs

The investment dependant costs are the decryption and the insurance.
The decryption per year is 10%, $0.1 * I_t$ = fl 10 million
The insurance is estimated on 1% per year, $0.01*I_t$ = fl 1 million
So K_i = fl 11 million.

6.3.4 Total operating costs per year

The total operating costs per year (K_t) are equal to $1.05*(K_p+K_l+K_i)$ = fl 147 million

6.4 Sales income

In Coulson [7] typical prices for bulk purchases, mid 1992 are found. These are prices for technical/industrial grade materials. For methanol the price is 0.7 £/kg. In 1992 1£=+/- 3.00.
So the total income (X) is 735 million.
In contradiction with this price is the value found in Callis [4] of 270 /ton.
Then the total income of 94.5 million is much to low and further calculations are not necessary! So for the rest of the calculations Coulsons value is used.

6.5 Return on investment

The net cash flow after taxes per year W is equal to the sales income minus the operating costs and taxes. So W=1/2*(X-Kt)

The return of investment (ROI) is equal to:

$$ROI=W/(It+Iw)*100\% \qquad (39)$$

with Iw is the working capital.
This working capital is estimated on 20% of the operating costs, so
Iw = 0.2*Kf = fl 29.4 million.
This gives

W=1/2*(735-147)= 294 million

ROI= 294/(100+20)*100=245%

6.6 Internal rate of return

For calculating the internal rate of return (IRR) the following equation has to be solved for i:

$$I_t+I_w=W/(1+i)+W/(1+i)^2+....W/(1+i)^9+(Iw+W)/(1+i)^{10} \qquad (40)$$

with IRR=100*i

For the calculated figures this gives IRR=245%

6.7 Economic evaluation

When Coulson is true the overall conclusion must be that this is a very good market at the moment.
When the Calis is true this project can be eliminated for this location.
In the last case it becomes very important what price is paid for the natural gas, because it is the determining factor of the profitability of the process.

In the early seventies natural gas was dumped at low prices because nuclear energy seemed to be the future and a lot of methanol plants were build. In [1] a price of fl 6 / GJ is paid, nowadays fl 8.21 /GJ. That leads to a difference of fl 21.6 million in the product volume costs! Nowadays natural gas is more expensive and it becomes important to make use of long term gas contracts. Also it has to be studied if its cheaper to have an own oxygen plant.

Chapter 7 Conclusions and recommendations

A methanol plant was developed with a production of 380,000 metric tons (12.07 kg/s) per year. The goal of 350,000 metric tons is reached. The methanol is 98,8 % pure. The impurity was mainly caused by dimethylether which was difficult to remove.

The reformer is operated autothermal, which was one of the goals of this assignment.
The autothermal process is achieved due to intensive heat integration. As a result the plant has a lot of large heat exchangers. The investment costs will be higher, but no furnace is needed so heating costs are cut down. The reformer without a furnace is a lot smaller then a conventional type of reformer. This also cuts down costs.

The investments costs of the plant are fl 100 million (rough estimation). The sales income of the methanol depends strongly on the methanol price used (of course). Using the price according to Coulson [7] the methanol sales income is fl 735 million per year. This would mean that the investment is earned back within one year. The plant is very profitable. Using the price according to Calis [4] the methanol sales income fl 94.5 million. The net cash flow becomes below zero, the process wouldn't be profitable. No clear view of the economics is gained. It is recommendable to make a long term deal with the natural gas suppliers for low prices because natural gas is the main operating cost

It is shown that the autothermal reforming is theoretically possible. Therefore it is recommended to carry out experiments on lab scale. These experiment will show whether or not the right chemical- and reactor kinetics are used.

It is also possible to include an oxygen plant in the design. It could profitable because of the large amount of oxygen which is used. The natural gas cleaning can also be included.

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Appendix A Mass and enthalpy flows

	mass flow [10^3 kg / s]				
stream number	1	2	3	4	5
component					
carbon dioxide	0	0	0	1234	1234
carbon monoxide	0	0	0	14005	14005
dimethyl ether	0	0	0	0	0
ethanol	0	0	0	0	0
hydrogen	0	0	0	2122	2122
methane	8911	0	8911	446	446
methanol	0	0	0	0	0
nitrogen	109	0	109	109	109
oxygen	0	8889	0	0	0
water	0	0	0	50246	50246
total	9020	8889	9020	68162	68162

	enthalpy flow [kW]				
stream number	1	2	3	4	5
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-41631	-2	-35339	-635028	-625014

	mass flow [10^3 kg / s]				
stream number	6	7	8	9 H_2O	10
component					
carbon dioxide	1234	1234	12	0	0
carbon monoxide	14005	14005	0	0	0
dimethyl ether	0	0	0	0	0
ethanol	0	0	0	0	0
hydrogen	2122	2122	0	0	0
methane	446	446	0	0	0
methanol	0	0	0	0	0
nitrogen	109	109	0	0	0
oxygen	0	0	0	0	0
water	50246	50246	50141	105	105
total	68162	68162	50153	105	105

	enthalpy flow [kW]				
stream number	6	7	8	9	10
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-829361	-865667	-796028	-1668	-1723

	mass flow [10^3 kg / s]				
stream number	11	12	13	14	15
component					
carbon dioxide	12	12	12	12	1223
carbon monoxide	0	0	0	0	14005
dimethyl ether	0	0	0	0	0
ethanol	0	0	0	0	0
hydrogen	0	0	0	0	2122
methane	0	0	8911	8911	446
methanol	0	0	0	0	0
nitrogen	0	0	109	109	109
oxygen	0	0	0	0	0
water	50246	50246	50246	50246	105
total	50258	50258	59278	59278	18010

	enthalpy flow [kW]				
stream number	11	12	13	14	15
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-797694	-662944	-698278	-638722	-69622

	mass flow [10^3 kg / s]				
stream number	16	17	18	19	20
component					
carbon dioxide	1223	1223	6674	6674	6674
carbon monoxide	14005	14005	25569	21223	21223
dimethyl ether	0	0	657	820	820
ethanol	0	0	10	335	335
hydrogen	2122	2122	4791	4167	4167
methane	446	446	4109	4109	4109
methanol	0	0	265	4560	4560
nitrogen	109	109	10	335	335
oxygen	0	0	0	0	0
water	105	105	108	298	298
			42193		
total	18010	18010	43255	43255	43255

	enthalpy flow [kW]				
stream number	16	17	18	19	20
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-62907	-58472	-165625	-169675	-176044

	mass flow [10^3 kg / s]				
stream number	21	22	23	24	25
component					
carbon dioxide	6674	6674	6674	6674	6674
carbon monoxide	21223	16978	16978	12903	12903
dimethyl ether	820	978	978	1131	1131
ethanol	335	653	653	957	957
hydrogen	4167	3558	3558	2973	2973
methane	4109	4109	4109	4109	4109
methanol	4560	8753	8753	12778	12778
nitrogen	335	1072	1072	1072	1072
oxygen	0	0	0	0	0
water	298	484	484	663	663
	42521		43259	43260	
total	43255	43255	43255	43255	43255

	enthalpy flow [kW]				
stream number	21	22	23	24	25
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-181636	-185672	-197578	-200958	-196523

	mass flow [10^3 kg / s]				
stream number	26	27	28	29	30
component					
carbon dioxide	6674	6674	6057	5451	5451
carbon monoxide	12903	12903	12849	11564	11564
dimethyl ether	1131	1131	730	656	656
ethanol	957	957	12	10	10
hydrogen	2973	2973	2966	2669	2669
methane	4109	4109	4071	3664	3664
methanol	12778	12778	295	265	265
nitrogen	1072	1072	1071	963	963
oxygen	0	0	0	0	0
water	663	663	3	3	3
total	43255	43255	28054	25245	25245

	enthalpy flow [kW]				
stream number	26	27	28	29	30
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-238722	-247064	-129203	-116281	-116281

	mass flow [10^3 kg / s]				
stream number	31	32	33	34	35
component					
carbon dioxide	5451	606	617	617	38
carbon monoxide	11564	1285	54	54	0
dimethyl ether	656	73	400	400	120
ethanol	10	1	946	946	931
hydrogen	2669	297	7	7	0
methane	3664	407	38	38	0
methanol	265	29	12483	12483	12162
nitrogen	963	107	2	2	0
oxygen	0	0	0	0	0
water	3	0	660	660	655
total	25245	2805	15207	15207	13906

	enthalpy flow [kW]				
stream number	31	32	33	34	35
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-104233	-12920	-117861	-117933	-108122

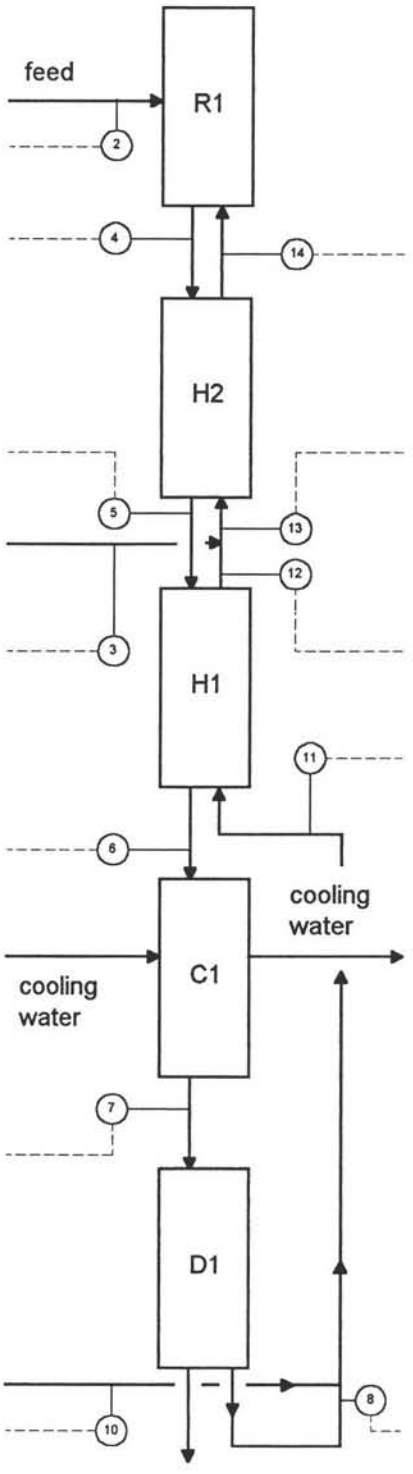
	mass flow [10^3 kg / s]				
stream number	36	37	38	39	40
component					
carbon dioxide	579	0	38	0	38
carbon monoxide	54	0	0	0	0
dimethyl ether	280	0	120	0	120
ethanol	15	9	922	913	9
hydrogen	7	0	0	0	0
methane	38	0	0	0	0
methanol	321	122	12040	120	11920
nitrogen	2	0	0	0	0
oxygen	0	0	0	0	0
water	5	649	7	7	0
total	1301	780	13127	1040	12087

	enthalpy flow [kW]				
stream number	36	37	38	39	40
component					
carbon dioxide					
carbon monoxide					
dimethyl ether					
ethanol					
hydrogen					
methane					
methanol					
nitrogen					
oxygen					
water					
total	-8823	-11086	-80322	-6372	-74908

Fabrieks Voorontwerp no. 3119

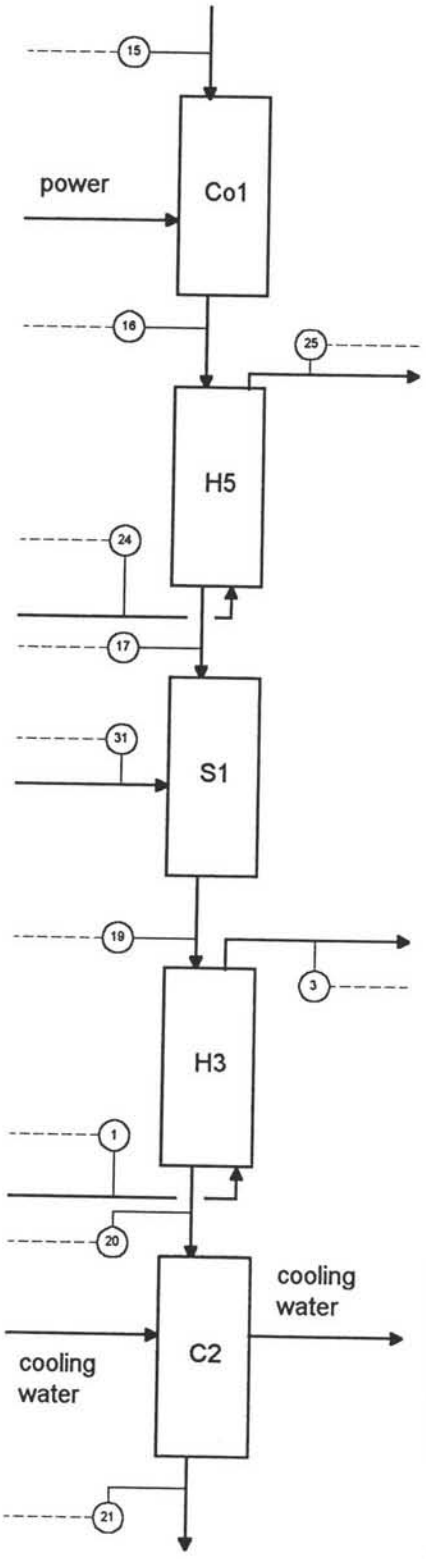
Appendix B **Mass and enthalpy balance**

IN		forward
M	-H	M
		-H
8.89	2	
		68.16
		635,028
		68.16
		625,014
9.02	35,339	
		68.16
		829,361
375.31	5,966,944	
		68.16
		865,667
		0.11
		1,666



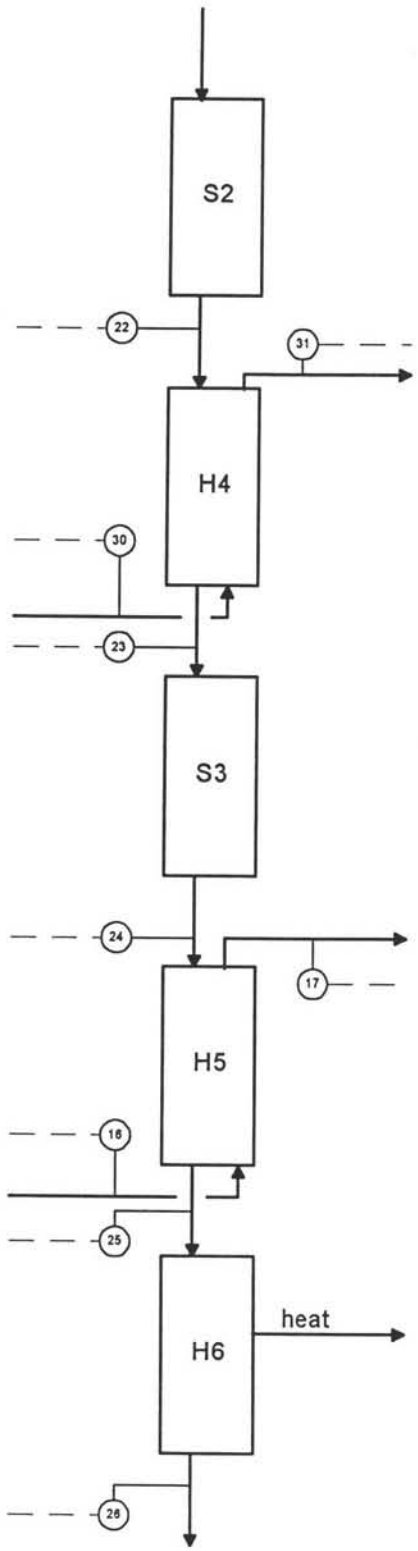
retour	OUT	
M	M	-H
-H		
59.28		
638,722		
59.28		
698,278		
50.26		
662,944		
50.26		
797,694		
	375.31	5,930,555
50.15		
796,028		

IN		forward
M	-H	M
		-H
		18.01
		69,622
	-6,715	
		18.01
		62,907
43.26	200,958	
		18.01
		58,472
25.25	104,233	
		43.26
		169,675
9.02	41,631	
		43.26
		176,044
125.1	1,988,9	
	72	
		43.26
		181,636



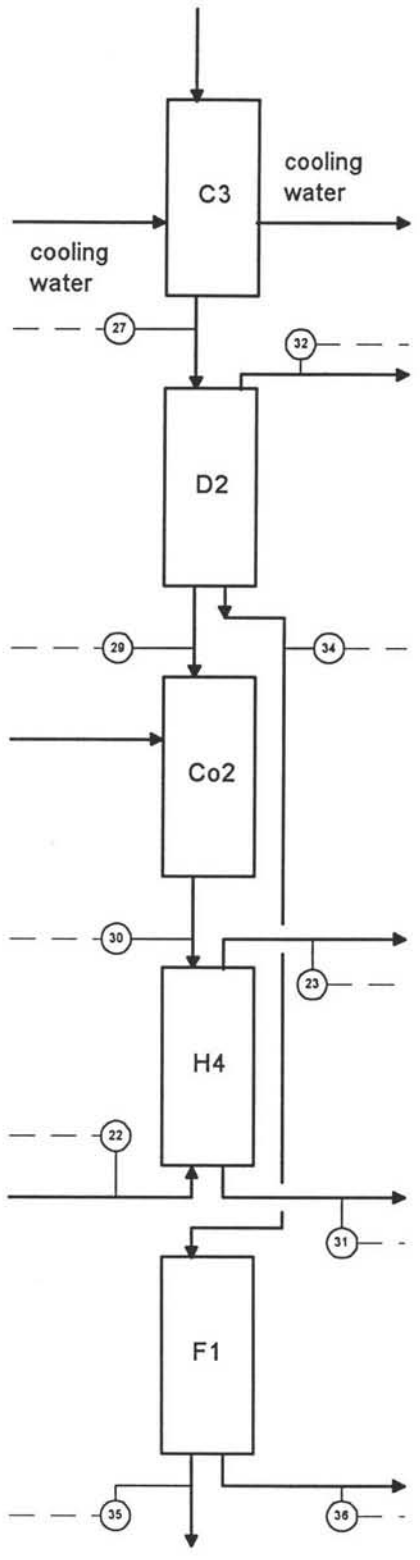
retour	OUT	
M	M	-H
-H		
	43.26	196,523
	9.02	35,339
	125.1	1,980,6
		11

IN		forward
M	-H	M
		-H
		43.26
		185,672
25.25	116,139	
		43.26
		197,578
		43.26
		200,958
18.01	62,907	
		43.26
		196,523
		43.26
		238,722



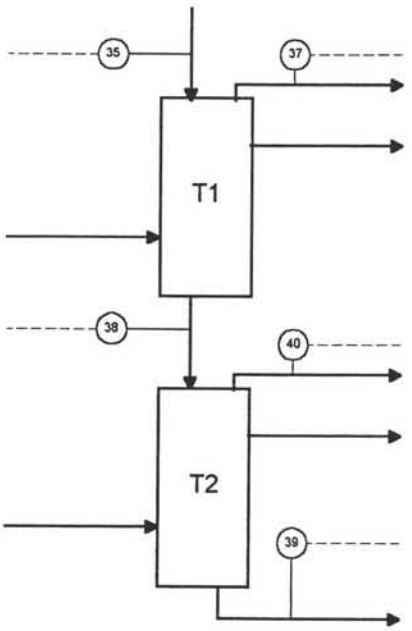
retour	OUT	
M	M	-H
-H		
	25.25	104,233
	18.01	58,472
		-42,199

IN		forward
M	-H	M
		-H
125.1	1,988,9	
	72	
		43.26
		247,064
		25.25
		116,281
	0	
		25.25
		116,281
43.26	185,672	
		13.91
		108,122



retour	OUT	
M	M	-H
-H		
	125.1	1,980,6
		11
	2.81	12,920
15.21		
117,933		
	43.26	197,578
	25.25	104,233
	1.3	8,823

IN		forward
M	-H	M
		-H
		13.91
		108,122
	-42,199	
		13.13
		80,322
	-26,759	
807.47	10,616,096	**total**



retour	OUT	
M	M	-H
-H		
	0.78	11,086
		-19,529
	12.09	74,908
		-27,717
	1.04	6,372
total	807.58	10,612,891

Mass in kg / s
Enthalpy in kW

Appendix C: List of equipment

Apparatenlijst voor reactoren, kolommen en vaten

APPARAAT NO.	R1	S1	S2	S3	
Benaming Type	Reformer	First bed synth.reac	Sec. bed synt.reac	Third bed synt.reac	
Abs. druk [bar]	10	100	100	100	
Temp [K]	1000	500	500	500	
Inhoud [m^3] Diameter [m] L of H [m]	 1.87 6.57	12.5	13.1	15.8	
Vulling: Schotels (+ aantal) Vaste pakking Kat. type Kat. vorm _____ _____ _____	 nickel rodd bundle	 MK101(=Cu/ Zn) packed bed	 MK101 packed bed	 MK101 packed bed	
Speciaal te gebruiken materiaal					
Aantal in - serie - parallel	 1 1				
Overig					

FABRIEKSVOORONTWERP NO. 3119

Apparatenlijst voor warmtewisselaars en fornuizen

APPARAAT NO.	H1	H2	H3	H4	H5
Benaming Type	Water heater	Ref. feed heater	Gas feed heater	recycle heater	Reac.feed heater
Medium - pijpen - mantel-zijde	water synthesis gas	water+methane synthesis gas	methane methanol/ synth.gas	synth.gas methanol/ synth.gas	syth.gas methanol/ synth.gas
Capaciteit Uitgewisselde warmte [kW]	1.58e4 + 1.48e4 (per h-e)	1.19e4 (per h-e)	2.26e4	4.3e4	1.60e4
Warmtewisselend oppervlak [m^2]	978 + 894	879	934	917	715
Aantal - serie - parallel	1 + 8 1 + 1	5 1	1 1	1 1	1 1
Abs. druk [bar] - pijpen - mantel-zijde	10 10	10 10	10 100	100 100	100 100
Temp. in/uit [K] pijpzijde mantelzijde	300/460 639/389	474/900 1010/639	300/560 570/517	300/470 570/470	380/470 570/531
Speciaal te gebruiken materiaal					
Overig					

FABRIEKSVOORONTWERP NO. 3119

Apparatenlijst voor warmtewisselaars en fornuizen

APPARAAT NO.	H6	H7	C1	C2	C3
Benaming Type	Destill. reboiler	Destill. reboiler	Reformer prod.cool	Reactor cooler	methanol cooler
Medium - pijpen - mantel-zijde	methanol methanol	methanol steam	synth.gas /water cooling water	methanol/ synth.gas cooling water	methanol/ synth.gas cooling water
Capaciteit Uitgewisselde warmte [kW]			1.81e4 per h-c	2.01e4	3.0e4
Warmtewisselend oppervlak [m^2]			646	35	433
Aantal - serie - parallel			2 1	1 1	1 1
Abs. druk [bar] - pijpen - mantel-zijde			10 3	100 3	100 3
Temp. in/uit [K] pijpzijde mantelzijde	531/350		389/300 293/313	517/470 293/313	350/300 293/313
Speciaal te gebruiken materiaal					
Overig					

FABRIEKSVOORONTWERP NO. 3119

Apparatenlijst voor warmtewisselaars en fornuizen

APPARAAT NO.	C4	C5			
Benaming Type	Condensor	Condensor			
Medium - pijpen - mantel-zijde	Methanol coolin water	methanol cooling water			
Capaciteit Uitgewisselde warmte [kW]					
Warmtewisse-lend opper-vlak [m^2]					
Aantal - serie - parallel					
Abs. druk [bar] - pijpen - mantel-zijde					
Temp. in/uit [K] pijpzijde mantelzijde					
Speciaal te gebruiken materiaal					
Overig					

FABRIEKSVOORONTWERP NO. 3119

Apparatenlijst voor reactoren, kolommen en vaten

APPARAAT NO.	F1	T1	T2	D1	D2
Benaming Type	Flash drum	Distill. column	Distill. column	Condensate drum	Condesate drum
Abs. druk [bar]	1	1	1	10	100
Temp [K]	310	338/356	337/348	300	300
Inhoud [m^3] Diameter [m] L of H [m]		 0.95 15	 2.0 18.5		
Vulling: Schotels (+ aantal) Vaste pakking Kat. type Kat. vorm _____ _____ _____		 28	 35		
Speciaal te gebruiken materiaal					
Aantal in - serie - parallel					
Overig					

Apparatenlijst voor pompen, blowers en compressoren

APPARAAT NO.	Co1	Co2	P1	P2	
Benaming Type	Intermediate cooled compressor	Compressor	Water feed pump	Water pump	
Te verpompen medium	Synthesis gas	Synthesis gas	Water	Water	
Capaciteit [kg/s]					
Dichtheid [kg/m^3]			1000	1000	
Zuig-/pers-druk (abs.) [bar]	10/100	90/100	7/10		
Temp. [K] in/uit	300/380	300/310	300/300		
Vermogen [kW] - theorie - praktijk	1.4e4 2e4				
Aantal - serie - parallel					
Speciaal te gebruiken materialen					
Overig					

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: H1 a

Aantal serie : 1
Aantal parallel :

Algemene eigenschappen

Type	: - warmtewisselaar		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 1.58e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 978	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 300	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 54	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		synthese gas	water
Massastroom	[kg/s]	68.12	50.26
Massastroom te			
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]		
Temperatuur IN	[K]	404	300
Temperatuur UIT	[K]	389	375
Druk	[bar]	10	10
Materiaal		Stainless steel	Stainless steel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum: 21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: H1 b

Aantal serie : 8
Aantal parallel :

Algemene eigenschappen

Type	: - warmtewisselaar		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 1.48e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 894	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 200	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 83	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		synthese gas	water
Massastroom	[kg/s]	68.12	50.26
Massastroom te			
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]		
Temperatuur IN	[K]	639	375
Temperatuur UIT	[K]	404	460
Druk	[bar]	10	10
Materiaal		Stainless steel	Stainless steel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: H2

Aantal serie : 5
Aantal parallel :

Algemene eigenschappen

Type	: - warmtewisselaar		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 1.19e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 879	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 100	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 135	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		water+methanol	synthesis gas
Massastroom	[kg/s]	68.12	50.26
Massastroom te			
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]		
Temperatuur IN	[K]	1010	474
Temperatuur UIT	[K]	639	900
Druk	[bar]	10	10
Materiaal		Stainless steel	Stainless steel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: H3

Aantal serie : 1
Aantal parallel :

Algemene eigenschappen

Type	: - warmtewisselaar		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 2.26e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 934	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 100	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 67.3	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		methanol/ synthesis gas	methane
Massastroom	[kg/s]		
Massastroom te		43.2	9.02
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]		
Temperatuur IN	[K]		
Temperatuur UIT	[K]	570	300
		517	560
Druk	[bar]		
Materiaal		100	10
		Stainless steel	Stainless steel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: H4

Aantal serie : 1
Aantal parallel :

Algemene eigenschappen

Type	: - warmtewisselaar		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 4.3e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 917	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 100	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 130.6	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		methanol/ synthesis gas	synthesis gas
Massastroom	[kg/s]		
Massastroom te		43.25	25.25
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]		
Temperatuur IN	[K]	570	300
Temperatuur UIT	[K]	560	470
Druk	[bar]	100	100
Materiaal		Stainless steel	Stainless steel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: H5

Aantal serie : 1
Aantal parallel :

Algemene eigenschappen

Type	: - warmtewisselaar		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 1.6e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 715	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 100	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 124.0	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		methanol/ synthesis gas	synthesis gas
Massastroom	[kg/s]		
Massastroom te		43.25	18.01
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]		
Temperatuur IN	[K]	570	380
Temperatuur UIT	[K]	531	470
Druk	[bar]	100	100
Materiaal		Stainless steel	Stainless steel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: C1

Aantal serie : 2
Aantal parallel :

Algemene eigenschappen

Type	: - Koeler		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 1.81e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 646	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 1000	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 28.06	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		cooling	watersynthesis gas/water
Massastroom	[kg/s]		
Massastroom te			68.16
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]	293	389
Temperatuur IN	[K]	313	300
Temperatuur UIT	[K]		
Druk	[bar]		
Materiaal		3 Stainless steel	10 Cupro-nickel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: C2

Aantal serie : 1
Aantal parallel :

Algemene eigenschappen

Type	: - Koeler		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 2.01e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 35	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 800	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 194.7	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		cooling	watersynthesis gas/methanol
Massastroom	[kg/s]		
Massastroom te			68.16
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]	293	517
		313	470
Temperatuur IN	[K]		
Temperatuur UIT	[K]		
Druk	[bar]		
Materiaal		3	100
		Stainless steel	Cupro-nickel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER WARMTEWISSELAAR

APPARAATNUMMER: C3

Aantal serie : 1
Aantal parallel :

Algemene eigenschappen

Type	: - Koeler		
Uitvoering	: - met vaste pijpplaten		
Positie	: - horizontaal		
Capaciteit	: 3.0e4	[kW]	(berekend)
Warmtewisselend oppervlak	: 433	[m^2]	(berekend)
Overall warmteoverdrachts-coëfficiënt	: 1000	[$W/m^2.K$]	(globaal)
Logaritmisch temperatuursverschil (LMTD)	: 19.2	[K]	
Aantal passages pijpzijde	: 1		
Aantal passages mantelzijde	: 1		
Correctiefactor LMTD (min. 0.75)	:		
Gecorrigeerde LMTD	:	[K]	

Bedrijfscondities

		Mantelzijde	Pijpzijde
Soort fluïdum		cooling	watersynthesis gas/methanol
Massastroom	[kg/s]		
Massastroom te			43.25
- verdampen	[kg/s]		
- condenseren	[kg/s]		
Gemiddelde soortelijke warmte	[kJ/kg.K]		
Verdampingswarmte	[kJ/kg]	293	350
		313	300
Temperatuur IN	[K]		
Temperatuur UIT	[K]		
Druk	[bar]		
Materiaal		3	100
		Stainless steel	Cupro-nickel

FABRIEKSVOORONTWERP NO. 3119

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER TORENS

APPARAATNUMMER : T1____

Algemene eigenschappen

Functie : - destillatie

Type toren : - schotel

Type schotel : - zeefplaat

Aantal schotels
- theoretisch :
- practisch : 28

Schotelafstand (HETS) : 0.5 [m] ----- Materiaal schotel : Stainless steel

Diameter toren : 0.95 [m] ----- Hoogte toren : 15 [m]

Materiaal toren : Stainless steel

Verwarming : reboiler

Bedrijfscondities

	Voeding		Top		Bodem		Reflux-/ Absorptie-middel		Extractie-middel
Temp. [K]	310		338		356		338		
Druk [bar]	1		0.99		1.1				
Dichtheid [kg/m^3]									
Massastroom [kg/s]	13.9		13.1		0.78				
	mol%	wt%	mol%	wt%	mol%	wt%	mol%	wt%	
Samenstelling									
Methanol		88		92		15			
Water		48		0.05		83			

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Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

Datum:21/12/94
Ontwerpers:

SPECIFICATIEFORMULIER TORENS

APPARAATNUMMER : T2____

Algemene eigenschappen

Functie : - destillatie

Type toren : - schotel

Type schotel : - zeefplaat
Aantal schotels
- theoretisch :
- practisch : 35
Schotelafstand (HETS) : 0.5 [m] ----- Materiaal schotel : Stainless steel
Diameter toren : 2.0 [m] ----- Hoogte toren : 18.5 [m]
Materiaal toren : Stainless steel
Verwarming : reboiler

Bedrijfscondities

	Voeding		Top		Bodem		Reflux-/ Absorptie-middel		Extractie-middel
Temp. [K]	338		337		348		337		
Druk [bar]	1		0.99		1.1				
Dichtheid [kg/m^3]									
Massastroom [kg/s]	13.1		12.08		1.04				
	mol%	wt%	mol%	wt%	mol%	wt%	mol%	wt%	
Samenstelling									
Methanol		92		98.7		11			
Ethanol		7		9		88			

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Appendix E Calculation of efficiency

$$E = \frac{3}{Mt}\left[\frac{1}{\tanh(Mt)} - \frac{1}{Mt}\right]$$

$$Mt = R_b\sqrt{K_s \frac{Sv}{D_{eff}}}$$

$$K_s = k^* \frac{RT}{S_g * 60 * 1.013e5}$$

$$D_{eff} = \frac{\varepsilon}{\tau}\left[\frac{1}{D_{m,\,mix}} + \frac{1}{D_{m,\,kn}}\right]$$

$$D_{m,\,mix} = \left[\sum_{i=2}^{n} \frac{x_i}{D_{CH_4,i}}\right]^{-1}$$

$$D_{CH_4,i} = 1.013e-7 * T^{1.75} * \left(\frac{\sqrt{\frac{M_{CH_4} + M_i}{M_{CH_4} * M_i}}}{P * \left(V_{CH_4}^{\frac{1}{3}} + V_i^{\frac{1}{3}}\right)^2}\right)$$

$$Vi = 1.98*\#H + 16.5*\#C + 5.48*\#O$$

$$Dm,kn = \frac{4}{3} d_{pore} * \sqrt{\frac{RT}{2\pi M_{CH_4}}}$$

$$d_{pore} = \frac{4 * \theta * Vp}{S_p}$$

E	=	efficiency
Mt	=	Thiele modules
Rb	=	radius of rod bundle
k	=	constant of the reaction
Deff	=	efficient diffusion coefficient
Dm,mix	=	diffusion of methane in the gas mixture
Dm,kn	=	Knudsen diffusion coefficient
R	=	gas constant
T	=	temperature
Sv	=	specific surface per volume
Sg	=	specific surface per mass
Vi	=	molecular volume of component i
Mi	=	molecular weight of component i
dpo	=	diameter of pore
ε	=	bed porosity
θ	=	particle porosity
τ	=	tortuosity
Vp	=	volume of the particle

Appendix F Compound characteristics

table F1: Enthalpy-related data

compound	H_0	$Cp/R=a+b*T+c*T^2+d/T^2$ [T in K]			
	[kJ]	a	b /1e-3	c/1e-6	d/1e5
CH_4	-74	1.7	9.08	-2.16	0
CO	-110	3.38	0.56	0	-0.03
CO_2	-393	5.48	1.05	0	-1.16
H_2	0	3.25	0.42	0	0.08
O_2	0	3.64	0.51	0	-0.23
$H_2O_{(l)}$	-241	3.47	1.45	0	0.12
$CH_3OH_{(l)}$	-200	2.21	12.22	-3.45	0
C_2H_5OH	-235	3.52	20	-6	0
N_2	0	0.59	0.59	0	0.04

table F2: Critical data

compound	T_c[K]	P_c[bar]	ω
CH_4	190.6	46	0.01
CO	132.9	35	0.05
CO_2	304.2	73.8	0.23
H_2	33.2	13	-0.22
O_2	154.6	50.5	0.02
H_2O	647.3	220.5	0.34
CH_3OH	512.6	81	0.56
C_2H_5OH	516.2	63.8	0.64
N_2	126.2	33.9	0.04

table F3: relevant Antoine-constants

compound	Antoine: $\ln(P)=A-B/(T+C)$; P[mmHg]; T[K]			H_{vap} [kJ]
	A	B	C	
H_2O	18.3	3,816.44	-46.13	40.68
CH_3OH	18.59	3,626.55	-34.29	35.28

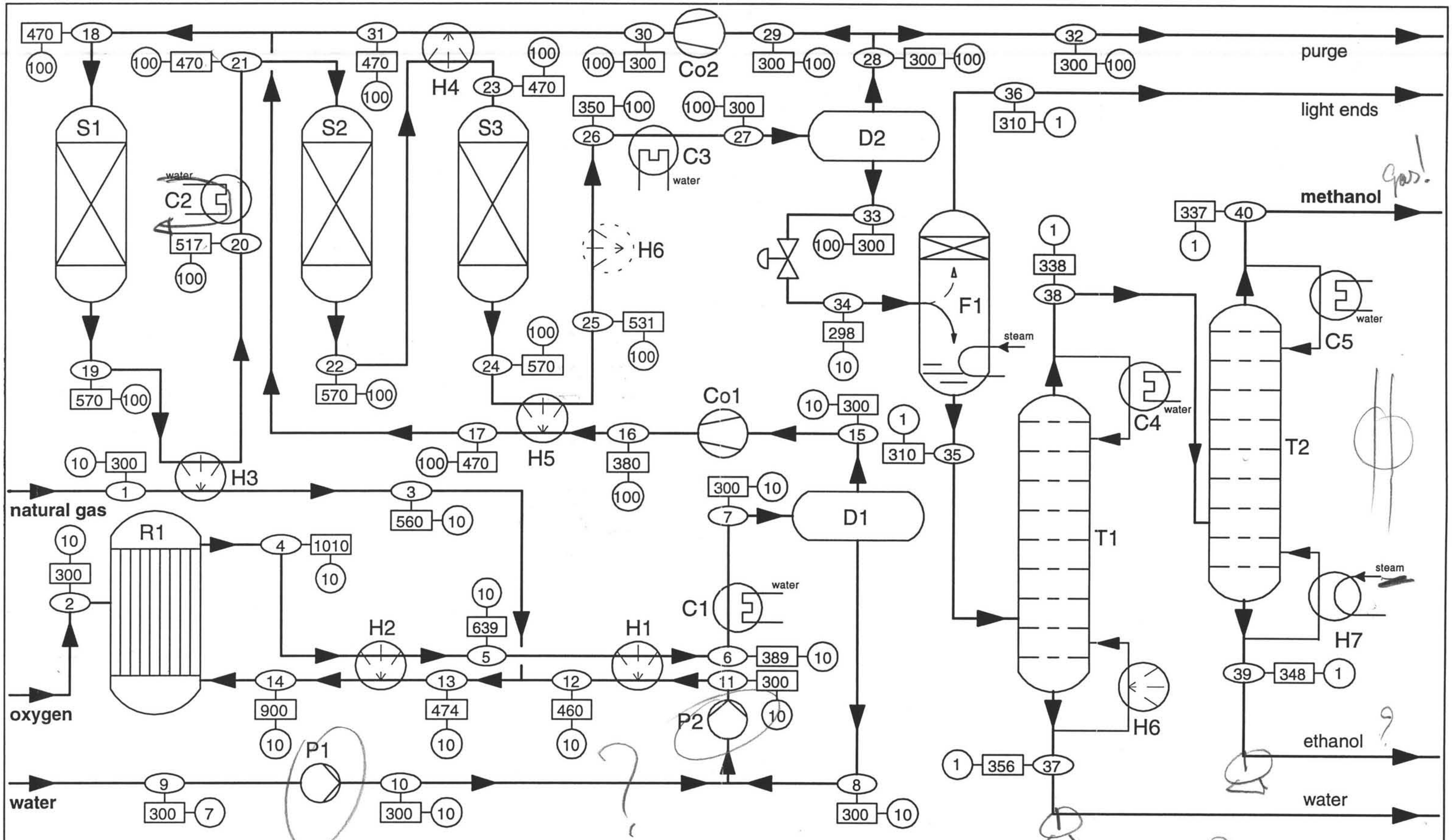
table F3 : general data

compound	mol wt	bol point [K]	rel desity water = 1	rel vap density air = 1	solubility in water
hydrogen	2.01	14.01		0.07	not
nitrogen	28.01	77.35		0.97	not
carbon monoxide	28.01	81.65		0.97	not
oxygen	32.00	90.12		1.1	10 mg/l at 20C
methane	16.04	109.15		0.6	not
carbon dioxide	44.01	194.65	0.8	1.5	16 mg/l at 25C
dimethyl ether	46.07	248.15	0.7	2.1	completely
methanol	32.04	338.30	0.8	1.1	completely
ethanol	46.07	351.65	0.8	1.6	completely
water	18.01	373.15			

table F4 : safety data

compound	explosion limits vol % in air	flash point	vap. pressure 293 K; 1 bar	$T_{ignition}$ [K]	MAC val. ppm
hydrogen	4 - 76	flammable gas			
nitrogen					
carbon monoxide	12 - 75	flammable gas	58.8	878	50
oxygen					
methane	5 - 16	flammable gas		810	
carbon dioxide			57.6		5,000
dimethyl ether	2.0 - 10.1	flammable gas	1.66	463	
methanol	5.5 - 36.5	11°C	0.127	728	200
ethanol	3.4 - 19	12°C	0.06	643	1,000
water					

Appendix G Flowsheets



C	cooler
Co	compressor
D	condensate drum
F	flasher

H	heat exchanger
R	reformer
S	synthesis reactor
T	distillation tower

flowsheet methanolsynthesis

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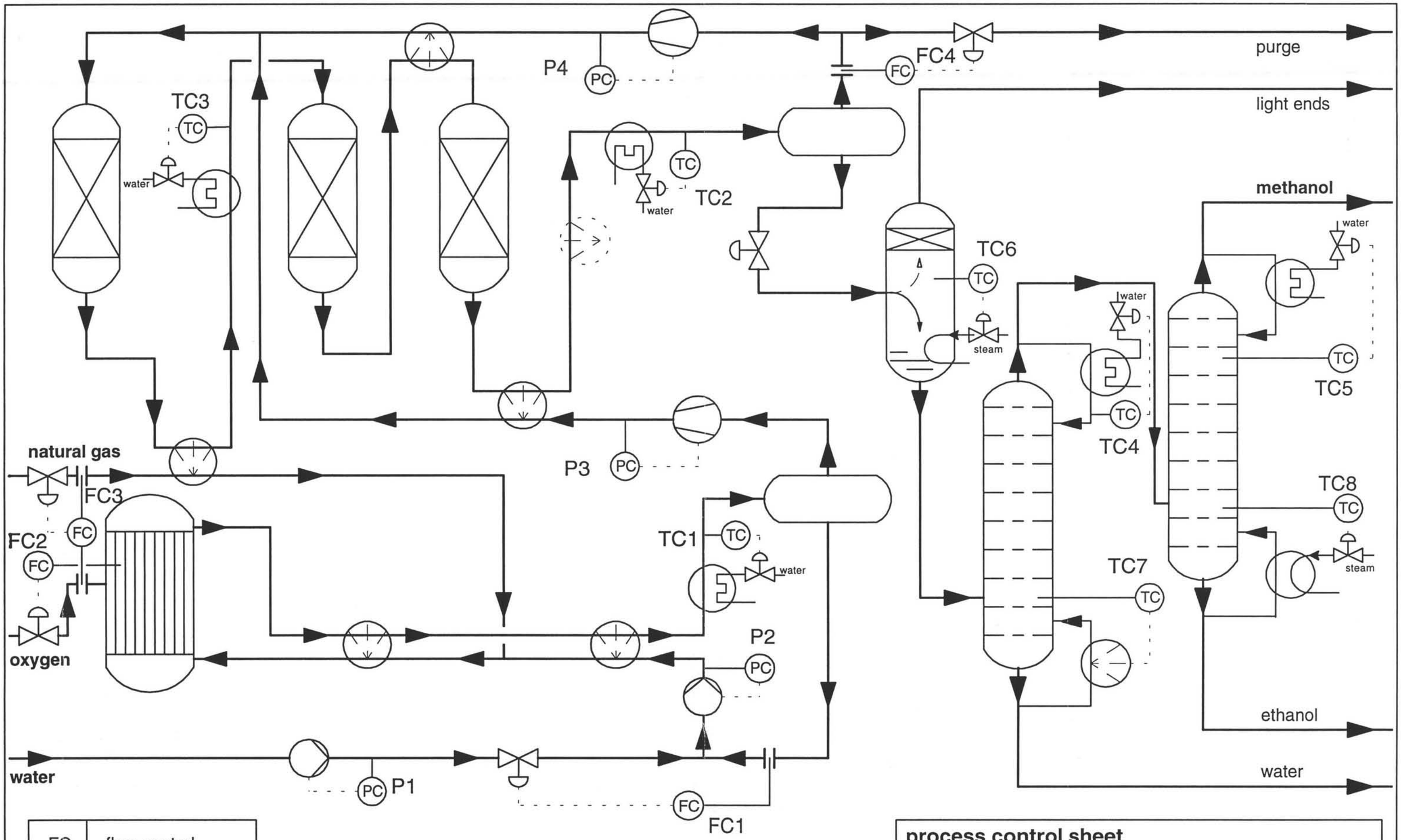
December 1994

Stream number | Temp. in K | Abs. pressure in bar



FC	flow control
P	pressure control
TC	temperature control

process control sheet
methanolsynthesis

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