FVO Nr. 3206

Preliminary Plant Design
Dept. of Chemical Process Technology

Subject

The production of methoxy-propanol and methoxy-propoxy-propanol from propylene oxide and methanol

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Keywords

Propylene glycolethers, Solvents, Propylene oxide, Methanol, Methoxy-propanol, Methoxy-propoxy-propanol, Homogeneous Catalysis

Date of assignment : September 16th 1997
Date of report : January 5th 1998

TU Delft
Technische Universiteit Delft

Faculteit der Scheikundige Technologie en der Materiaalkunde

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Summary

The main objective of this process predesign is to design a profitable plant that produces 85,000 t/a 1-methoxy-2-propanol (MP-2) and 15,000 t/a methoxy-propoxy-propanol (MDP) from methanol (MeOH) and proylene oxide (PO). The product specification for MP-2 is >99.9 %w with < 0.01 %w methanol and < 0.1 %w of its isomer MP-1. The purity of MDP has to be >99.0 %w with < 0.1 %w MP-1.

The products belong to the group of the proylene glycolethers. Applications of MP-2 in particular are pharmaceutical, cosmetic, cleaning and degreasing, crop protection and painting inks and coatings. The applications for MDP are the same except for the pharmaceuticals and cosmetics.

As mentioned before methanol and propylene oxide react to MP-2. However also the formation of an unwanted by-product, 2-methoxy-1-propanol (MP-1), takes place. MP-1 and PO react to MDP in a second reactor section. Sodiummethylate ($NaOCH_3$) is used as the homogeneuos base catalyst for the reactions. The selectivity of this catalyst towards MP-2 is over 90%.

The plant describes a continuos process and is designed for an annual onstream period of 50 weeks and is made up of two resembling reactor sections which consist of a reactor followed by two distillation columns. The ~~design is~~ based on a German patent from January 1997.

Figure A below shows the process flow diagram.

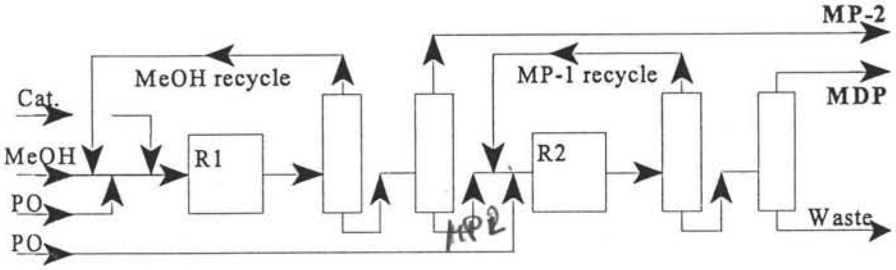

Figure A: Process flow diagram

In the first reactor section the production of MP-2 takes place. The excess amount of methanol fed to the reactor is separated from the products in the first distillation column and is recycled to the reactor. In the second distillation column MP-2 is separated from MP-1. MP-1 is fed to the second reactor where it reacts to MDP. The surplus amount of MP-1 leaves the next column over the top and is recycled to the reactor. MDP is recovered in the fourth distillation column. The bottom stream consists of catalyst and heavier propylene glycolethers. This waste stream amounts 2,957.89 t/a. The two reactors are multitubular plug flow reactors; the distillation columns are sieve plate columns.

The economic lifetime of the plant is assumed to be 15 years. To estimate the economics of the process Lang's factorial method has been used. The total investment of the project is 14,212 kfl[illegible], the total operating costs are 171,524 kfl/a. The price of MP-2 and MDP is 1824 fl/t. This results in a net profit of the plant -from start-up- of 10,929 kfl/a. The Pay-back Time (PBT) is 4 years and 4 months; the Rate of Return (ROR) is 63.56%.

Acknowledgements

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Contents

1. Introduction

Propylene oxide (PO) is one of the major intermediates in the chemical industry. Almost all PO produced is converted into derivatives like polyether polyols (polyurethanes), propylene glycols and propylene glycolethers.

Propylene glycolethers are formed by the reaction of propylene oxide and alcohols, like methanol and ethanol. Certain traditional ethylene glycolethers and their acetates are being replaced by their PO-based analogues. The main reason for this replacement is the (suspected) toxicity of some of the glycolethers based on ethylene oxide (EO). Therefore the market for propylene glycolethers is growing relatively fast.

Propylene glycolethers constitute the third largest market for PO-based derivatives (5 %). World production of propylene oxide was 3200 ktonnes per year in 1992, with an expected annual growth of 4 %. As a result, the market for propylene glycolethers constitutes approximately 350 ktonnes per year [28].

Propylene glycolethers are used in a broad variety of applications, like solvents in varnishes, inks and paints, but can also be encountered as heat transfer fluids or anti-icing agents. The powerful dissolving characteristic of glycolethers and their esters, combined with their generally low volatility, is the basis of their main function as solvents.

Important propylene glycolethers are methoxy-propanol and methoxy-propoxy-propanol. The first one being the replacement for its toxic EO-based counterpart. Applications of methoxy-propanol can be found in pharmaceutics and cosmetics, as well as in cleaning, degreasing, crop protection, painting inks and coatings. Methoxy-propoxy-propanol shows the same applicative properties except for pharmaceutics and cosmetics.

The design focuses on the production of 100 ktonnes per year methoxy-propanol (MP-2) and methoxy-propoxy-propanol (MDP) out of the raw materials propylene oxide and methanol. The required production rates are 85 ktonnes per year MP-2 and 15 ktonnes per year MDP.

The process is simulated with the flowsheeter ChemCad.

2. Basis of Design

Conceptual Process Design.

The assignment for this preliminary plant design is to design a process that converts methanol and propylene oxide into the desired products 1-methoxy-2-propanol (MP-2) and methoxy-propoxy-propanol (MDP). The design is based on a German patent from 1997 [25]. The specifications of the desired products are given in Table 2.1. In Appendix C.1 an overview of the substances in the process is presented.

Product	Production rate (ton/a)	Purity (%w)	Impurities (%w)
MP-2	85,000	>99.9 >99.89	< 0.1 MP-1 and < 0.01 MeOH
MDP	15,000	>99.0 >99.9?	< 0.1 MP-1

< 0.11

Table 2.1: Product specification list.

2.1. Reactions and Reaction Mechanism

The process comprises of two reactor sections as will be discussed in section 2.2. The first reactor is dedicated to production of MP-2, while in the second reactor MP-1, the toxic and thus unwanted isomer of MP-2, reacts with PO to MDP. The following sections will give more insight in the reaction mechanism and in the main reactions taking place.

2.1.1. Reactions

As mentioned before, the main product forming reactions to MP-2 and MDP are performed in separate reactors. The product forming reactions are listed below whereas a complete overview of all reactions taken into account is listed in appendix C2 :

MP-1

$\rightarrow CH_3OCH(CH_3)CH_2OH$

MP-2 reaction

$$\underset{MeOH}{CH_3OH} + \underset{PO}{CH_3CH(O)CH_2} \rightarrow \underset{MP\text{-}2}{CH_3OCH_2CH(CH_3)OH} \qquad [1]$$

$\Delta H_r = -98.36$ kJ/mol at 157°C

MDP reaction

$$\underset{MP\text{-}1}{CH_3OCH(CH_3)CH_2OH} + \underset{PO}{CH_3CH(O)CH_2} \rightarrow \underset{MDP}{CH_3OCH_2CH(CH_3)OCH_2CH(CH_3)OH} \qquad [2]$$

$\Delta H_r = -112.58$ kJ/mol at 177°C

All reactions occurring are first order in the key-component propylene oxide.

2.1.2. The Reaction Mechanism

The reaction mechanism for the formation of propylene glycolethers comprises of several parallel and series reactions. Essentially, the highly reactive propylene oxide reacts with hydroxyl groups in the various (intermediate) reactants like methanol or MP-2. Due to the structure of PO, cleavage of the oxirane ring leads to the formation of two isomers out of each reactant. All these isomers, having a newly formed hydroxyl group from the oxirane ring, can react further with PO. This reaction mechanism results in a mixture of isomers of various propylene glycolethers. Therefore, the product distribution is a function of input variables like the molar ratio of reactants and temperature. In Appendix C.2 the reaction mechanism for the formation of propylene glycolethers as well as the formation of propylene glycols is outlined..

2.2 Catalyst Selection

The reactions mentioned in section 2.1.1. can be catalysed in different ways. The possible ways to catalyse the reactions are thermic, by an acid, by a base or by zeolites. In selecting the catalyst, criteria like selectivity towards desired products (e.g. MP-2 instead of MP-1), conversion and cost of the catalyst were taken into account.

A homogeneous base is used as catalyst in the process. Base catalysts are known for their good selectivity towards one of two isomers. In this case selectivity towards MP-2 instead of MP-1 is over 90 per cent. Moreover, this type of catalysts can be obtained rather cheap.

Thermic catalysis is not desirable, because the temperature has to be high in order to start up the reactions. Besides, high temperatures may cause decomposition of the products to, for instance, aldehydes. With the use of an acid catalyst, equal amounts of MP-2 and MP-1 are formed. Therefore, acid catalysts are not considered as an option. The selectivity of the zeolite catalysts towards MP-2 is very high but conversion is too low (only 40 per cent). Moreover, zeolites are expensive.

The homogeneous base used in the process is sodiummethylate ($NaOCH_3$). The selectivity of this catalyst towards MP-2 is over 90%. Selectivity towards MP-2 of other base catalyst, like tertiary amines, is slightly better, but they are much more expensive than sodiummethylate.

Commonly used as base catalyst is sodiumhydroxide (NaOH). A negative effect of this catalyst with respect to the reactants is the direct reaction of the hydroxyl-ion OH^- with PO. As a result, valuable reactant is lost to unwanted propylene glycols. Moreover, it is very likely that difficulties will occur with achieving the required specifications of the products. This is especially true for MDP, because dipropylene glycol and MDP have almost the same boiling point. With sodiummethylate as catalyst this problem will not occur, because the methanolate-ion (CH_3O^-) is actually methanol in ionized form. Therefore $NaOCH_3$ was chosen as a catalyst. A positive side effect of this catalyst is a slightly better selectivitiy than NaOH towards MP-2 instead of MP-1. Although sodiummethylate is more expensive than sodiumhydroxide, the advantages mentioned above justify the choice for sodiummethylate as catalyst..

2.3 Hierarchial Approach

In this section a hierarchial approach described by Douglas (1988) will be used to define the assignment and to explain the process choices made.

The process essentially comprises of a reaction section, in which MeOH and PO are converted into the products, and a separation section to purify the products. Due to the nature of this process, the dedicated production of 100 ktonnes per year, a continuously operated process scheme is chosen. Figure 2.1 gives a block diagram for this process.

Fig. 2.1: Block diagram input-output structure

As shown in the block diagram above the input-output structure is straight forward. The reactants enter the process whereas desired products and some by-products leave the process.

The recycle structure of the process depends on the choice of a reactor configuration. For the reaction section two configurations can be distinguished. The main product forming reactions can be performed in one or two reactors. Due to the difference in reaction rates of the two main reactions, it is more favourable to use two reactors instead of one. The underlying reasons in favour of the two-reactor configuration are:

- two smaller reactors instead of one large reactor
- no need for very large recycle flows to push reactions towards desired products
- more flexible operation optimised for the main reaction taking place in the reactor.

When focusing on the main reactions taking place, the recycle structure becomes clear.
In the first reactor the conversion of MeOH and PO to MP-2 and inevitably its isomer MP-1 takes place. In the second reactor the unwanted MP-1 and fresh PO is converted to MDP. It was found that excess amounts of MeOH and MP-1 in the first, respectively second reactor are necessary to achieve the desired production rates. Thus recycling of the surplus of MeOH and MP-1 is evident.

This reasoning leads to the conclusion that the separation section consists of at least a recycle column and a product column for each reactor. For the one-reactor configuration the same kind of reasoning leads to a distillation train comprising of at least two recycle columns and two product columns. The following process diagram for the two reactor configuration becomes clear.

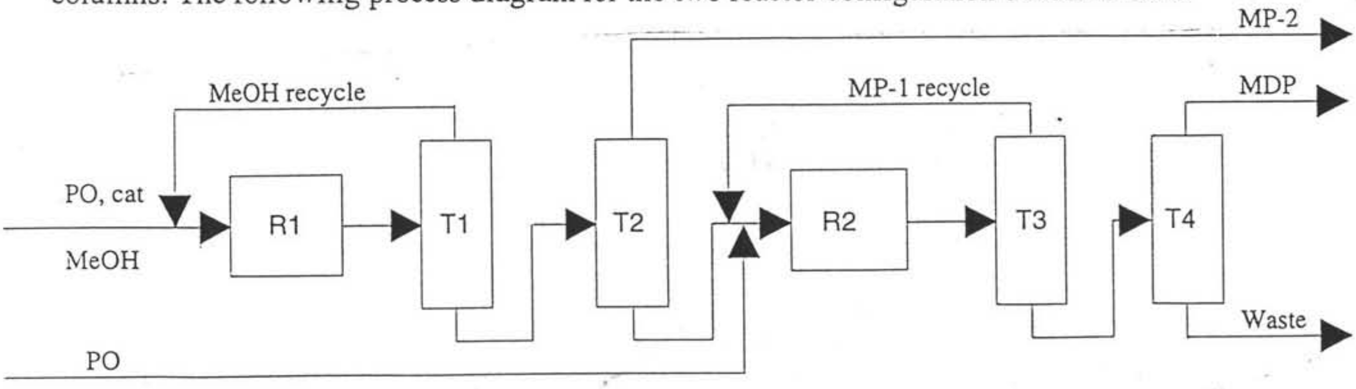


Fig. 2.2: Process flow diagram

2.4 Battery Limit

Essentially, the flow diagram of Fig.2.2 describes the process and its equipment within the battery limit. For this process the following equipment is taken into account:

- MP-2 reactor
- MDP reactor
- The recycle columns
- The product columns
- Heat transfer equipment
- Pumps
- Valves

Production of utilities, waste treatment and storage facilities are not considered within the battery limit.

Feed streams are fed to the process at 1.3 bar and 20°C. The compositions of the various feed streams are tabulated below.

Cat.

Stream numbers	**1 (kg/h)**	**2 (kg/h)**	**3 (kg/h)**	**4 (kg/h)**
Methanol	114	3928.3	-	-
Propylene oxide	-	-	7377	800
Water	-	3.9283	-	-
$NaOCH_3$	38	-	-	-

Table 2.2: Feed stream compositions

The product streams leave the process at elevated pressure (2 bar) and 60°C in order to store the products properly in tanks.

2.5 Utilities

The utilities available to meet heating and cooling requirements are steam and cooling air. The conditons for steam are given in Table 2.3

	LP steam	**MP steam**
P (bar)	4	18
T (°C)	200	320
T^{sat} (°C)	143.6	207.1

Table 2.3: Steam conditions

Cooling water cannot be used in this design, because the total cooling water capacity is already used. Instead of cooling water, air is used. The design air temperature is set at 23 °C.

Electricity is used at either 220 V or 380 V.

2.6 Lifetime and Site Location

The lifetime of the plant is assumed to be fifteen years.

The plant is situated in the Botlek industrial area nearby the Port of Rotterdam, according to the assignment. The raw materials needed for this process are eas~~y~~ accesible and transportation by ×
road, water and rail is rather easy.
ily

2.7 Market demand

Propylene glycolethers constitute the third largest market for PO-based derivatives (5 %). World production of propylene oxide was 3200 ktonnes per year in 1992, with an expected annual growth of 4 %. As a result, the market for propylene glycolethers constitutes approximately 350 ktonnes per year. The market is growing relatively fast due to the replacement of (suspected) toxic EO-based glycolethers with their PO-based counterparts. = 5%

2.8. List of components

On the next page an overview of all used components and some of their properties is presented in Table 2.4.

Table 2.4 List of Components

	mol. formula	*mol. weight (kg/kmol)*	*boiling point* [(1)] *(°C)*	*melting point* [(1)] *(°C)*	*liq. density* [(2)] *(kg/m³)*	*liq. viscosity* [(2)] *(mPa·s)*	*MAC value (ppm)*	*explosion limits (%v/v)*	*auto ignition temp. (°C)*
1,2-Propyleneoxide PO	C_3H_6O	58.081	✓ 34.2	-11.9	829.6	0.314	100	1.9-39.0	430
Methanol MeOH	CH_4O	32.042	✓ 64.7	-97.7	794.3	0.575	200	5.5-36.5	455
Water H_2O	H_2O	18.015	✓ 100.0	0.0	996.3	1.033			
1-Methoxy-2-propanol MP2	$C_4H_{10}O_2$	90.122	✓ 120.1	-96.7	923.8	1.913	100	1.5-13.7	290
2-Methoxy-1-propanol MP1	$C_4H_{10}O_2$	90.122	✓ 130.0		938.0				
Propyleneglycol PG	$C_3H_8O_2$	76.095	✓ 187.6	-60.0	1036.4	55.320			
Methoxy-propoxy-propanol MDP	$C_7H_{16}O_3$	148.202	188.3	-80.0	954.1	11.810			
Dipropyleneglycol DPG	$C_6H_{12}O_3$	134.175	✓ 213.8	-40.2		112.127			
Methoxy-dipropoxy-propanol MTP	$C_{10}H_{22}O_4$	206.283	✓ 242.4	-42.0	970.4	39.437			
Methoxy-tripropopxy-propanol M4P	$C_{13}H_{28}O_5$	264.363	✓ 408.3						
Sodiummethylate S	$NaOCH_3$	54.024	✓						

(1) Boiling point and melting point at atmospheric pressure
(2) Liquid density and viscosity at 20°C

3. Process Structure

In this chapter the structure of the process and a detailed description of the various unit- operations and operating conditions is given. The following section will give more insight in the process structure.

3.1 Process Description

In this section the process flowsheet (Appendix A) will be discussed. Together with the mass and heat balance (Appendix B1) and the list of stream compositions (Appendix B2), the process flowsheet will give a good overview of the process. Essentially, the flowsheet shows two reaction sections with a distillation section for each reaction section. The first reaction section produces methoxy-propanol (MP-2), whereas the second reaction section methoxy-propoxy-propanol (MDP) produces.

3.1.1. MP-2 Reaction Section

The feed streams enter the process at 1.3 bar and 20°C. The catalyst stream (1), methanol recycle stream (5) and fresh feed streams (2 +3) are separately pressurized to 27.5 bar in order to keep reactants liquid at reaction temperature. The great excess amount of volatile methanol makes this necessary. Methanol and propylene oxide feed streams are mixed up thoroughly with the recycle methanol stream from the the methanol recycle column (T7).

Before entering the reactor (R5), the mix-up stream of reactants (11) should be heated in order to start reaction.The heat of reaction is used to preheat the feed streams from 55°C to 140°C. Just before entering the reactor the mix-up stream (12a) and the catalyst stream (6) are mixed, initiating reaction. The reactor is not operated isothermally, but under a temperature profile. The reactor outlet temperature is 152°C, while the maximum temperature reached in the reactor is 170°C.

The effluent is depressurized to 1 bar over a control valve before entering the recycle methanol distillation column (T7). Excess methanol, residual PO and water leave the top of the column while product leaves as bottom stream (recycle ratio: 1.8). In the second column (T12) MP-2 leaves the top as product with a purity of over 99.9 % w. The bottom stream (17) of the MP-2 column contains primarily in ~~great extent~~ MP-1, MP-2 and some higher propylene glycolethers and propylene glycols. After repressurizing to 13 bar, this stream enters the second reaction section, where MDP is produced.

3.1.2. MDP Reaction Section

The second reaction section resembles the first reaction section in most aspects. In comparison with the first section two features are changed. First, the fresh PO stream is not mixed with the bottom stream of the second column untill the reactor inlet is reached. Otherwise reaction will probably already take place at the shell-side of the reactor, due to the presence of catalyst in the bottom stream. Second, the pressure needed to keep reactants liquified is moderate, 13 bar; as result of the presence of heavy and less volatile components and the absence of MeOH in the bottom stream.

After repressurizing the recycle stream (20) of the MP-1 column (T21) to 13 bar, the bottom stream of the second column (21) and the recycle stream are mixed thoroughly. The fresh PO stream (4) is also pressurized to 13 bar. First, the mix-up stream of reactants (21) is cooled to 100°C. As a consequence, the heat capacity of the stream is large enough to be preheated to 170°C. Just in front of the reactor inlet, both feed streams are mixed together and reaction is started. As was the case in the first reaction section, the reactor is operated under a temperature profile. The maximum temperature reached during reaction is 200°C. The temperature at the reactor outlet is 174°C.

After reaction, the more volatile components like MP-1, MP-2 and PO leave the recycle MP-1 column (T21) as top products. The top stream is recycled to the reactor (recycle ratio: 2.4). The bottom stream of the column is led to the MDP purifying column (T28). MDP leaves the column as top stream with a purity of over 99.0 %w. The bottom stream (29) constitutes a mixture of heavy propylene glycolethers like MDP and MTP, and catalyst. To prevent crystillization from occurring in the column, it is important that the Na^+ concentration in the bottom stream does not exceed 5 %w.

The product streams (18, 29, 30) are cooled to 60°C and kept at 2 bar to prevent leakage of oxidizing air into the system. Under these conditions, the product streams are ready to be stored in storage tanks.

3.2 Thermodynamics and Kinetics

In the next section the thermodynamics and kinetics of the process are described. Especially kinetics have a great influence on both reactors in the system as will be shown later.

3.2.1. Thermodynamics

For the simulation to be reliable and give good results it is very important to select a proper thermodynamic model. First a choice has to be made wether to use an activity-coefficient method or an equation of state model.

Activity-coefficient methods are being used when, among others:
- a liquid is (strongly) non ideal
- polar components are present
- electrolytes are present

Equations of state are preferred to be used when:
- super critical components are present
- operation condition is near critical
- the system consists of: normal fluids (CH, N_2, O_2 etc.), light polar components or CO_2, H_2S, H_2

The operating conditions and components present, do meet the requirements for an activity-coefficient method to be used much better than for an equation of state.

Since the so called UNIFAC method is an activity-coefficient method that accounts for a wide range of components and conditions this method is the one used to simulate the system.

ly

New defined components.

ly

The components MP-1 and M4P had to be new-defined for they were not in the simulation program's database. The thermodynamic properties needed for a good simulation, like heat capacity and heat of formation, of these components have been calculated by the Benson group-contribution method [1]. This Benson method is a reliable method that can be used for a wide range of compounds.

3.2.2. Kinetics

As was mentioned earlier, the reactions comprise of a number of series and parallel reactions simultaneously. In Appendix D all reactions taken into account and their kinetic data are listed. The following assumptions about the reactions were made:

will leave system with HE's

- the reaction to M4P has the same kinetics as the reaction to MTP.
- reactions to higher propylene glycolethers than M4P were not considered because only small amounts of M4P were formed.
- reactions to propylene glycols have the same kinetics as reaction to MP-2.
- reactions higher than DPG were not considered; only small amounts of DPG were formed.

All reactions occurring are first order in the key-component propylene oxide. The activation energy (E_A), the pre-exponential constant (k_0) and thus reaction rate vary with each reaction. The reaction rate is given by the Arrhenius relation:

$$k = k_0 \cdot \exp\left(-\frac{E_A}{R \cdot T}\right) \tag{3.1}$$

Because it provides

~~For~~ the only variable in this relation is the temperature T, ~~there lies~~ the clue in enhancing selectivity towards desired products. Dividing two reaction rates, gives the selectivity towards a certain product. Depending on the activiation energy E_A in both reaction rates, selectivity will be enhanced by either increasing or decreasing temperature. For example, selectivity towards MP-2 relative to MP-1 is favoured by lower temperature.

Two major limitations are connected with using temperature as a tool.Temperature can not be increased infinitely to enhance selectivity. In this case very high pressure should be applied to keep the reaction mixture liquid. Also product degradation can occur. To prevent product degradation in this design, temperature should not be higher than 200 °C.
On the other hand, if a low temperature is desirable, reaction rates will slow down. This implies ~~for~~ large reactors in order to get acceptable conversion.
~~The~~ limitations considered ~~above~~ fix the temperature range in which reactors should ~~be~~ operate~~d~~ efficiently.

still

above

3.3 Unit Operations

In the next sections the choices and conditions of unit operations are outlined.

3.3.1. Reactors

In general three types of reactors can be distinguished: batch reactors, continuous stirred tank reactors and plug flow reactors. Due to the nature of the process, continuous operation is desired, resulting in a choice between continuous stirred tank or plug flow reactors.

A plug flow reactor is the most suitable reactor for the process. The main reason for this choice is the fact that in a plug flow reactor the concentrations of the reactants stay high for a longer period of time than in a continuous stirred reactor. As a result the concentrations of the products stay low. This increases the selectivity towards MP-2 and MP-1 in the first reactor and the selectivity towards MDP in the second reactor. Another advantage af the plug flow reactor is the good heat exchanging capability. This is necessary since the occurring reactions are exothermic.
The reactors in this design serve two purposes. Beside serving as a regular plug flow reactor, the reactor serves as a heat exchanger. The feed stream is preheated at the shell-side of the reactor by the heat generated by reaction. To prevent reaction from starting too early, the catalyst stream in the first reaction section and the fresh PO feed stream in the second reaction section are mixed just in front of the respective reactor inlets with the respective preheated feed streams.

MP-2 reactor (R5) (156 -> 158°C)
The MP-2 reactor in the first reaction section is dedicated to the production of MP-2. Inevitably, MP-1 is produced. Selectivity towards MP-2 instead of MP-1 is favoured by low temperature. Dividing both rate constants leads to this result. It was found that 130°C is the minimum temperature at which reaction takes place at acceptable rate. The maximum temperature is set by the pressure needed to keep the reaction mixture liquid (excess amount of volatile methanol). It was found that 170°C was the maximum temperature reached during reaction, which corresponds to a pressure of 23 bar. This maximum temperature will be reached in the reactor due to the temperature profile that is allowed for.
Above 170°C, increasing temperature leads readily to a higher pressure needed to keep the reaction mixture liquid. This was not considered desirable. To allow for slight temperature changes, the operating pressure in the reactor was chosen at 27.5 bar.

MDP reactor (R19) (176 -> 178°C)
In the second reactor, MDP is produced mainly by reaction of MP-1 with PO. Unfortunately, MDP will react with PO to form MTP. Again, selectivitiy towards MDP will increase with lowering temperature. It was found that for sufficiently high reaction rates 165°C was the minimum temprature. The maximum temperature reached during reaction is 200°C. The operating pressure for this reactor was chosen as 13 bar.

3.3.2. Distillation Columns

In general three types of columns can be distinguished: plate columns, random packed columns and structured packed columns. The choice for a plate column was based on the main advantages and disadvantages listed in Coulson and Richardson page 530 and further [6].

- Plate columns can handle a wider range of gas and liquid flow rates.
- Plate columns can be designed with more assurance (otherwise liquid distribution is difficult to maintain, especially in large packed columns).
- It is easier to make provision for sidestreams from plate columns.
- Packed columns are often applied when plate diameter is less than 0.5 m for small plates can not be cleaned in a proper way through manholes.

Also three different types of plates can be distinguished: bubble-cap, valve plates and sieve plates (in order of descending price). In general, sieve plates are satisfactory for most applications. Valve plates are only used when the operating range can not be matched with sieve plates. Bubble caps have a positive liquid seal and can therefore operate at very low vapour rates. Because no special reasons were apparent for choosing the more expensive plates, sieve plates were chosen.

Separation is best when pressure is as low as possible. On the other hand, distillation beneath atmospheric pressure is expensive because vacuum has to be maintained. Therefore, if practically possible, atmospheric pressure was chosen as operating pressure.

3.3.3. Heat Exchangers

In absence of cooling water capacity, air is used to meet cooling requirements. For this purpose air-fan coolers were used to meet cooling requirements.
The reboilers of the distillation columns are designed with usage of the steam capacity available on site. The type of reboilers used in this design is the horizontal thermosyphon reboiler. If no high viscosity fluids are present or no near vacuum operation is necessary, a thermosyphon reboiler is an economical choice and suitable for most applications. Sufficient static head is needed to create the thermosyphon effect. Therefore, the total column should be elevated resulting in extra costs for the foundation. With horizontal thermosyphon reboilers this negative effect is smallest. Compared to vertical thermosyphons, horizontal thermosyphons are easier maintained, although more complicated piping is necessary.

3.3.4. Reducing Valves

All the valves used at the plant are control valves. This means that also the reduction of the pressure of the streams entering the first and the third distillation column will be regulated simply by control valves. These two automatic control valves are basically globe valves with special trim designs.

3.3.5. Pumps

The two main types of pumps are the positive displacement pump and the centrifugal pump. Centrifugal pumps are most widely used in the process industry. Their efficiency depends on the flow-rate to be pumped through and is about 30 to 40% for the given flow-rates. So, because the flow-rates of all the different streams are small (with a maximum of 33 m^3/h), and hence the efficiencies of the centrifugal pumps are low, positive displacement pumps are used throughout the plant. The positive displacement pumps used are all rotary pumps. They are able to deliver nearly constant rates and they are able to deliver against high pressures.

3.3.6. Mixers

For continuous mixing of low viscosity fluids, as is the case here, inline mixers can be used.

The mixing of the MeOH and PO feed streams of the first reactor with the MeOH recycle stream can be realized by using injection mixers, for the feed streams are much smaller than the recycle stream. Injection mixers are mixers in which the one fluid is introduced into the flowing stream of the other through a concentric pipe or an annular array of jets. Mixing will take place by entrainment and turbulent diffusion and will give a satisfactory blend in about 80 pipe diameters.

(R5)

The injections of MeOH and PO needed in the first reactor can occur close to each other. The catalyst, however, must be injected as close to the reactor inlet as possible to keep reactions from starting before entering the reactor. This will be done by injecting the catalyst into the feed stream of the reactor after it has been warmed up and letting it pass through a static mixer.

(T12)

The mixing of the bottom stream of the second distillation column with the MP-1/MP-2 recycle stream can also be realized by using an injection mixer. PO must be injected as close to the reactor inlet as possible, in the same way and for the same reason the catalyst must be injected as close to the first reactor inlet as possible.

4. Equipment Calculations

4.1 Reactors

In this section the design calculations for the reactor are made. The results of these calculations can be found in appendix E1.

4.1.1. MP-2 Reactor (R5)

The type of reactor
The reactor is a multitubular plug flow reactor. The reactions take place in the tubes and cooling takes place on the shell-side in order to remove the heat produced during the reactions. Since the feed must be heated before entering the reactor, the feed is used as the cooling medium.

The reactions
In the first reactor PO and MeOH react to mainly MP-2 and MP-1. The overall reaction is as follows:

$$PO + MeOH + H_2O \rightarrow MP{-}2 + MP{-}1 + MDP + MTP + M4P + PG + DPG$$

A kinetic reactor is modelled with ChemCad in order to calculate the required volume of the reactor and the product distribution. Although in practice the reactor is operated under a temperature profile, which will be explained later, the reactor modelled with ChemCad is an isothermal reactor at the mean reactor temperature. For the reactor design the conversion of the key component, PO, is said to be complete, so no PO leaves the reactor. The stoichiometric coefficients for the overall reaction are calculated with the results of the reactor simulated in ChemCad. The calculation of the coefficients is listed in Appendix E1.2.

See <13> ?

Mass balance
In order to calculate the conversion of the components in the reactor mass balances have to be made. PO is taken as the key component. The mass balance of PO can be described as follows:

$$\frac{dC_{PO}}{dV} = \frac{r_{PO}}{\phi_v} \tag{4.1}$$

In this equation the reaction rate of PO is determined by the kinetics of the reaction (Appendix D). For the other compounds similar equations can be obtained. These are mentioned in Appendix E1.1. The meaning of the symbols used in this chapter can be found in chapter 10.

Equation 4.1 can also be written in terms of the residence time in the reactor:

$$\frac{dC_{PO}}{d\tau} = r_{PO} \tag{4.2}$$

This has been done because of the different volumes of shell and tubes. The assumption is made that the residence times in shell and tube are equal. ?

Energy balance

The reactions that occur are exothermic so the heat of reaction has to be removed from the reactor. As mentioned above the cooling is done by sending the cold feed through the shell of the multitubular reactor.

The heat produced is the overall heat of reaction. The overall heat of reaction, ΔH_R is calculated by summation of the heats of formation of the compounds:

$$\Delta H_R = \Sigma \nu_i \Delta H_f \tag{4.3}$$

The heats of formation of the compounds and the overall heat of reaction can be found in Appendix E1.2. The heats of formation were either found in the literature [10 and 21] or calculated by the method of Benson [1]. With the overall heat of reaction and the conversion of the key component known, the total heat production can be calculated. The energy balance for the reaction mixture is:

$$\frac{dT}{d\tau} = \frac{-UA(T-T_{feed})/V - \nu_{PO} r_{PO}(-\Delta H_R)}{\Sigma C_{p,i} C_i} \tag{4.4}$$

Since cooling is done by the feed it is also necessary to write down an energy balance for the feed.The energy balance for the feed becomes:

$$\frac{dT_{feed}}{d\tau} = \frac{UA(T-T_{feed})/V}{\Sigma C_{p,i} C_i} \tag{4.5}$$

The mass balances and energy balances above were numerically solved with the computer program RRStiff (see Appendix E1.1 for the equations used). This led to the temperature profiles in the reactor of both the reaction mixture (T) and the feed (Tfeed).

From the temperature profile in Fig. 4.1 it can be seen that in the first part of the reactor the heat production is higher than at the end of the reactor. This is due to the fact that at the beginning the reactant concentrations are high and as a result the reaction rate is high and that causes much heat production. Because UA is constant over the entire length of the reactor, the reactor temperature will rise in the beginning of the reactor because the local heat transfer capacity is too low. At the end of the reactor the temperature will decrease because there the local heat capacity is too high. The heat produced during the reaction will be absorbed by the feed and for a small part by the reaction mixture itself.

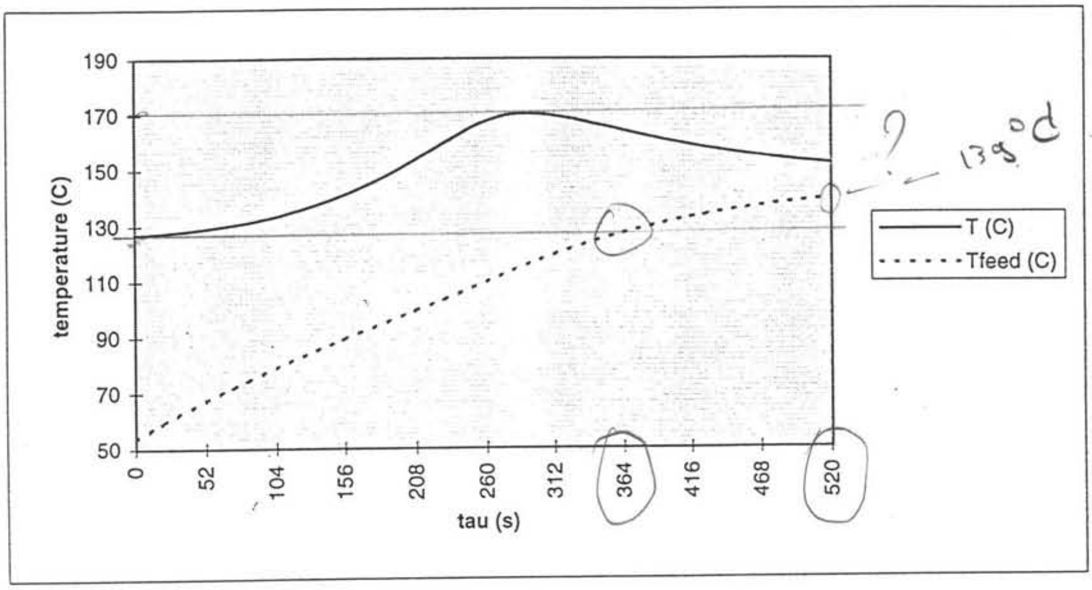


Fig. 4.1.Temperature profile for the first reactor R5

In order to create the right distribution between those two destinations for the heat of reaction the value of UA is varied. By the method of 'trial and error' an appropiate value for UA is found. Hereby it is taken into account that the maximum temperature in the reactor must not exceed 170 °C to avoid vaporization of the reaction mixture at the given pressure. On the other hand the feed must not reach an outlet temperature that is too high. The right value of UA in order to achieve both of these conditions is 60000 W/m²°C. However in this case the feed comes out of the shell at a temperature of 139 °C. That is still 12 °C too high but no heat exchanger was designed to cool this stream. A possible solution ~~for this difficulty~~ might be the removal of the feed from the shell, as soon as it has reached the right inlet temperature for the reactor. This will have as a consequence that the temperature in the reaction mixture will rise after removing the feed, due to a lack of cooling capacity.

Heat exchange in the reactor

The reactor can be seen as a shell and tube heat exchanger. Herefor, the design of the reactor follows the design of a shell and tube heat exchanger.
The heat duty, Q, of the reactor can be calculated with the following formula:

$$Q=UA\Delta T_m \tag{4.6}$$

where, Q=heat duty (W)
U=heat transfer coefficient (W/m²°C)
A=heat transfer area (m²)
ΔT_m=mean temperature difference (°C)

The mean temperature difference has been calculated by taking the mean value of 50 temperature differences from the temperature profile.

As mentioned above the value of UA is 60,000 W/m^2°C. To start the design calculations a global value for U is taken.There are tables and nomographes available in the literature. When the heat transfer coefficient,U, is known the heat transfer area, A, can be calculated.
An extra complexity in the design is the fact that the inner volume of the tubes must equal the reactor volume and the outer area of the tubes must equal the heat transfer area. Furthermore, the ratio of the cross flow area of the shell, $A_{cr,s}$, and the cross flow area of the tubes, $A_{cr,t}$, should be equal to the ratio of the volumetric flow in the shell and tubes respectively. This is because of the assumption that the residence time in the shell is equal to the residence time in the tubes. This leads to the following equations, which determine the value for the tube diameter:

$$A = N_t \pi d_o L \tag{4.7}$$

$$V = N_t \frac{\pi}{4} d_i^2 L \tag{4.8}$$

$$A_{cr,s} = A_{cr,t} \frac{\phi_{v,s}}{\phi_{v,t}} \tag{4.9}$$

$$A_{cr,t} = \frac{N_t \frac{\pi}{4} d_i^2}{N_p} \tag{4.10}$$

These equations determine the inner diameter of the tubes, the tube length and the number of tubes, as well as the required cross flow areas.

Once the tube diameter is known the reactor can be designed. The real value of the heat transfer coefficient can be calculated and compared to the original estimated value. During this procedure certain values like the baffle spacing and the tube pitch were varied in order to get the right crossflow area for the shell.

The expressions for the inside and outside fluid film coefficient are mentioned below. With these values and the values for the fouling factors, the overall heat transfer coefficient can be calculated.

$$h_o=(\frac{k}{d_e})j_H Re\,Pr^{0.33}(\frac{\mu}{\mu_w})^{-0.14} \tag{4.11}$$

$$h_i=(\frac{k}{d_i})j_H Re\,Pr^{0.33}(\frac{\mu}{\mu_w})^{-0.14} \tag{4.12}$$

$$\frac{1}{U}=\frac{1}{h_o}+\frac{1}{h_{od}}+\frac{d_o\ln(\frac{d_o}{d_i})}{2k_w}+\frac{d_o}{d_i}\cdot\frac{1}{h_{id}}+\frac{d_o}{d_i}\cdot\frac{1}{h_i} \tag{4.13}$$

When the design for the reactor is finished the pressure drop on both sides can be calculated by means of the two formulas below.

$$\Delta P_s=8j_f(\frac{D_s}{d_e})(\frac{L}{l_B})(\frac{\mu}{\mu_w})^{-0.14}\frac{\rho u_s^2}{2} \tag{4.14}$$

$$\Delta P_t=N_p(8j_f(\frac{L}{d_i})(\frac{\mu}{\mu_w})^{-0.14}+2.5)\frac{\rho u_t^2}{2} \tag{4.15}$$

Construction material

The reactor is made of carbon steel. This is cheap and available in a wide range of forms and sizes. The use of carbon steel is possible here because there are almost no corrosive compounds. Only the water that is in the MeOH is corrosive, present only in very low concentrations.

(R5)

The design results for the MP-2 reactor can be found in Table 4.1. The calculations can be found in Appendix E1.3.

Design item	**Value**
V (m^3)	7.0
A (m^2)	731.7
d_i (mm)	44
d_o (mm)	50
L (m)	10
N_t	466
D_s (m)	1.94
ΔP_t (Pa)	299
ΔP_s (Pa)	12

Table 4.1. Design results for the MP-2 reactor

4.1.2. MDP-Reactor (R19)

Type of reactor

This reactor is also a multitubular plug flow reactor. The design procedure for this reactor is similar to the design procedure for the first reactor and the results can be found in Appendix E1.

The reactions

The overall reaction in the second reactor is as follows:

$$PO + MP\text{-}2 + MP\text{-}1 + PG \rightarrow MDP + MTP + M4P + DP.G$$

The stoichiometric coeffcients for this reactor can be found in Appendix E1.2.

Mass and energy balance

The mass and energy balances can be found in Appendix E1.1. Here also the problem arises of finding the optimal value for UA. The temperature in the reactor must not exceed 200°C according to the voltalities of the components and the outlet temperature of the shell must not be too high. In this reactor the appropriate value for UA is 10,000 W/°C in order to keep the temperature in the reactor below 200°C. Originally, the feed temperature at the entrance of the shell is too high. In this way there is not sufficient cooling capacity and the outlet temperature of the feed will be too high. In order to prevent this, the feed is cooled by an air cooler before entering the shell-side of the reactor.

The temperature profile for the MDP reactor becomes:

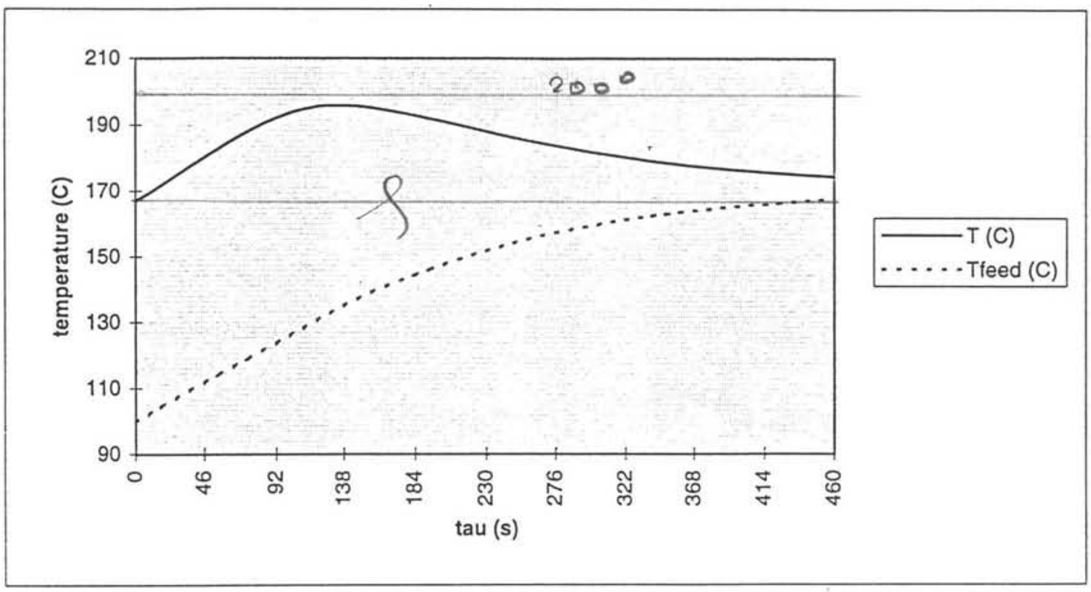


Fig. 4.2. Temperature profile reactor 2

Construction material
The MDP reactor is made of carbon steel, for the same reasons mentioned for the MP-2 reactor .

The design ~~results~~ for the MDP reactor are listed below in Table 4.2. The calculations can be found in Appendix E1.3

Design item	Value
V (m^3)	1.2
A (m^2)	122.0
d_i (mm)	45
d_o (mm)	50
L (m)	10
N_t	78
D_s (m)	1.00
ΔP_t (Pa)	361
ΔP_s (Pa)	24

Table 4.2. Design results for the MDP-reactor

4.2 Distillation Column Design

In the next sections the design procedure for a distillation column is described. The symbols used in the equations are given in section 10. The equipment calculations can be found in Appendix E2.1 and the results can be found in Appendix E2.2.

4.2.1. Design Considerations

The operating range is the range over which a plate can be operated efficiently. Outside this range plate efficiency will drop sharp and pressure drop will increase. The upper limit to vapour flow is set by the condition of flooding. Flooding is caused by either the excessive carry-over of liquid to the next plate by entrainment, or by liquid backing-up in the downcomers. The lower limit of the vapour flow is set by the condition of weeping. Weeping occurs when the vapour flow is insufficient to maintain a level of liquid on the plate.

In the following sections the different steps in designing the overall-column dimensions and interior dimensions is briefly described. In Appendix E2.1 an extensive overview of estimations and calculation results is given. The procedure used to design the distillation column is described in Coulson & Richardson (page 508 and further) [6].

4.2.2. Tower Design

The tower is divided into two sections, the top- or rectifying section and the bottom-or stripping section (with respect to the feeding stage). As a consequence the design of a distillation column falls apart in designing a plate for the rectifying and for the stripping section. The relationships for calculating both plates are the same.

The flooding condition fixes the upper limit of vapour velocity and thus the column diameter. High vapour velocity is needed for high plate efficiencies. Normally 85 per cent of the flooding velocity is taken as design value. The flooding velocity can be estimated from the correlation given by Fair:

$$u_f = K_1 \cdot \sqrt{\frac{\rho_l - \rho_v}{\rho_v}} \tag{4.16}$$

K_1 can be obtained from C&R and is correlated with the liquid-vapour flow factor F_{LV} in the following way:

$$K_1 \propto F_{LV} = \frac{\phi_{m,l}}{\phi_{m,v}} \cdot \sqrt{\frac{\rho_v}{\rho_l}} \tag{4.17}$$

To calculate the column diameter an estimate of the net area is required. This follows easily from the mass flow and the design value for flooding velocity calculated above. The net area, A_{net} must be corrected for the downcomer area in the columns.

Typically, 12 per cent of the total area is taken as initial design value. This leads to the following column diameter:

$$d_{col} = \sqrt{\frac{4}{\pi} \cdot A_{col}} \ , \quad with \ A_{col} = \frac{A_{net}}{1 - 0.12} \tag{4.18}$$

The next step is the design of a provisional plate. Coulson gives some methods to estimate parameters like weir dimensions, active area, hole area, hole size, the number of holes and the hole pitch.

With the results calculated and estimated above one still has to justify if the column will be practically operable. At first weeping is considered, then plate pressure drop, downcomer back-up and finally entrainment is checked.

Weeping

The lower limit of the operating range occurs when liquid leakage through the plate holes becomes excessive. The minimum design vapour velocity through the holes is given by:

$$u_{h,\min} = \frac{[K_2 - 0.90(25.4 - d_h)]}{(\rho_v)^{½}} \tag{4.19}$$

The hole diameter, d_h, was chosen arbitrarily in the provisional plate design. K_2 is a constant, depending on the depth of clear liquid on the plate (C&R).

The clear liquid depth equals the weir height h_w plus the crest of liquid over the weir h_{ow} . The latter can be estimated using the Francis weir formula for segmental downcomers:

$$h_{ow} = 750 \ [\frac{\Phi_{m,l}}{\rho_l . l_w}]^{⅔} \tag{4.20}$$

The weir length, l_w , is estimated with C&R.
Weeping will not occur if vapour velocity exceeds the required minimum vapour velocity.
Otherwise the provisional plate design has to be adjusted.

Plate pressure drop

The total plate pressure drop h_t, expressed in mm liquid, is as follows:

$$h_t = h_d + (h_w + h_{ow}) + h_r \ \text{resid.} \tag{4.21}$$

The dry plate pressure drop, h_d , is given by:

$$h_d = 51.[\frac{u_h}{C_o}]^2.\frac{\rho_v}{\rho_l} \tag{4.22}$$

C_o is called orifice coefficient and is a plate property; u_h is the hole velocity. The residual head h_r is given by:

$$h_r = \frac{12.5\times10^3}{\rho_l} \tag{4.23}$$

Downcomer back-up

The level of liquid and froth in the downcomer should be well below the top of the outlet weir on the plate above to prevent flooding. The downcomer liquid back-up (h_b) is defined as follows:

$$h_b = (h_w + h_{ow}) + h_t + h_{dc} \tag{4.24}$$

The head loss in the downcomer, h_{dc}, results from resistance to flow in the downcomer and can be estimated using the following equation:

$$h_{dc} = 166\ (\frac{\phi_{m,d}}{\rho_l . A_m}) \tag{4.25}$$

To account for the froth density in the downcomer, the liquid back-up (h_b) calculated from equation 4.24 should satisfy the following condition:

$$h_b < \frac{(l_t + h_w)}{2} \tag{4.26}$$

Finally, the residence time in the downcomer must be sufficient for the entrained vapour to disengage from the liquid stream. A residence time at least of 3 seconds is recommended. The residence time is given by:

$$t_r = \frac{A_d . h_b . \rho_l}{\phi_{m,d}} \tag{4.27}$$

Entrainment check

With the entrainment check the amount of liquid flowing with vapour is calculated. The flow factor F_{LV} is correlated with the fractional entrainment and the percentage flooding. Typically, the fractional entrainment should fall below 0.1 in order to neglect entrainment effects on plate efficiency. In the design plate efficiency is assumed to be 80 percent.

Design results

The column diameter, column height, number of trays are listed below in Table 4.3.

Equipment number	**Dcol (m) stripping section**		**Dcol (m) rectifying section**	**Column height (m)**	**N (real)**
T7	2.80		2.80	16.56	32
T12	3.00	6.07 *)	3.00	48.53	80
T21	0.85		1.30	22.14	35
T28	0.54		0.54	6.90	12

Table 4.3 Design results distillation columns

*) Though the relative volatility of MP-2 relative to MP-1 is almost constant throughout the entire column, the stripping section of column T12 shows an immense increase of the tray streams towards the bottom of the column. No possible explanation was found. The increase of the tray streams was met by enlarging the diameter of the bottom trays of the stripping section. In reality, different diameters in one section are not desired. A small change in the proces conditions or stream compositions changes the stream profile in the column which changes the separation. Using different diameters in one section makes it difficult to control the separation.

4.3 Heat Exchangers

4.3.1 General Relations for Heat Transfer

The results of the heat exchanger design can be found in Appendix E3.

The general equation for heat transfer across a surface is as follows:

$$Q = UA\Delta T_m \tag{4.6}$$

where, Q=heat duty (W)
U=heat transfer coefficient ($W/m^2 {}^\circ C$)
A=heat transfer area (m^2)
ΔT_m=mean temperature difference (°C)

One can find the true mean temperature difference by multiplying the logarithmic mean temperature difference (LMTD) by a correction factor, F_t.

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \frac{(T_1 - t_2)}{(T_2 - t_1)}} \tag{4.28}$$

$$\Delta T_m = F_t \Delta T_{lm} \tag{4.29}$$

The correction factor F_t is dependent on two dimensionless temperature ratios, R and S.

$$S = \frac{(t_2-t_1)}{(T_1-t_1)} \tag{4.30}$$

$$R = \frac{(T_1-T_2) \times C_p \times \phi_m}{(t_2-t_1) \times C_p \times \phi_m} \tag{4.31}$$

In the literature there are graphs available to determine the correction factor with known values of R and S (for instance Fig. 12.19 in Coulson and Richardson) [6].

The heat load of a stream can be calculated if one knows the heat capacity and the desired temperature difference :

$$Q = \phi_m C_p (T_{out} - T_{in}) \tag{4.32}$$

If a phase change (e.g. condensation or vaporization) occurs during heating or cooling the equation for the heat load becomes:

$$Q = \phi_m [C_p (T_{out} - T_{in}) + \Delta H_{vap}] \tag{4.33}$$

When designing a heat exchanger, one uses a global value of U. Reasonable values for the heat transfer coefficient can be obtained from Coulson and Richardson [ref. 21]. Then, with Q and the LMTD calculated from the equations above, the necessary heat transfer area can be calculated by equation 4.6.

4.3.2 Air Coolers

For the preliminary design of the air cooled heat exchangers the procedure recommended by Brown [ref. 4] is used. In this procedure certain assumptions were made. First, the approximate value of the heat transfer coefficient was determined by means of the table presented in the article. Second, the air temperature rise is calculated via an empirical formula. Furthermore the design is made for bare tubes, although in practice finned tubes will be used. The heat transfer area of a finned tube is assumed to be 15 times the heat transfer area of a bare tube of the same size.
The empirical formula for the air temperature rise is as follows:

$$(T_{air,out} - T_{air,in}) = \boxed{8.806 \cdot 10^{-4}} \, U \left[\frac{(T_{tubes,in} + T_{tubes,out})}{2} - T_{air,in}\right] \tag{4.34}$$

For this temperature rise a correction factor is needed which can also be obtained from the article by Brown. Once the temperature rise of the air is known the LMTD can be calculated and then the heat transfer area is known.

The fan power required for the air cooler was obtained from another article, Glass [ref. 16]. It is related to the heat transfer coefficient and the heat transfer area.

4.4 Pumps

Efficiencies
The efficiencies of the positive displacement pumps used is taken as 70%.

Pump shaft power
The power required for pumping an incompressible fluid is given by:

$$Power = \frac{\Delta P \ \phi_v}{\eta_p} * 100 \qquad (4.35)$$

where, ΔP = pressure differential across the pump, N/m^2,
ϕ_v = volumetric flow rate, m^3/s,
η_p = pump efficiency, %.

Power = Watts

The Table below shows the pump shaft power of all the pumps used at the plant, except for the pumps in the condenser sections of the different distillation columns.

Equip. No.	ΔP (N/m^2)	ϕ_v (m^3/s)	Theoretical power (kW)	Actual power (kW)
P1 Cat	26.200e5	4.436e-5	0.116	0.166
P2 MeOH	26.200e5	1.356e-3	3.553	5.075
P3 PO	26.200e5	2.427e-3	6.359	9.084
P4 PO	11.700e5	2.683e-4	0.314	0.448
P6 MeOHrec	26.487e5	7.766e-3	20.570	29.385
P14 T12 Btms	11.037e5	4.454e-4	0.491	0.702
P20 MMrec	11.987e5	1.689e-3	2.024	2.892
P27 MP2	6.870e4	3.221e-4	0.022	0.032
P35 MDP	7.020e4	5.186e-4	0.036	0.052
P36 HEk	5.940e4	9.583e-5	0.0056	0.008

Table 4.4 Pump shaft power

47.844

4.5 Utilities

The utilities consumed by the equipment consist of low pressure steam, middle pressure steam and electricity. The amounts of utilities neccessary for the plant are listed in Appendix E4.

5. Process Control

Instruments are provided to monitor and control the key variables during plant operation. These process control equipment are installed to ensure safe and stable operation of the plant. In this plant vife types of controllers are used: pressure controllers (PC), temperature controllers (TC), flow controllers (FC), level controllers (LC) and speed controllers (SC).

5.1 Process stability

For process control and product specification garantee the plant is provided with control equipment. In this section the way the different process units are controlled is described.

5.1.1 Reactors

Constant pressure and temperature in the reactors are essential to ensure the stability of the process. Since the feed streams of the reactors are first warmed up by reacting streams through the tubes of the reactors, the heat exchange within the reactors is between two process streams whose flows are fixed. Therefore, a by-pass control will be used to control the temperature. The temperature of the cooling stream will be measured at some point (or points) in the reactor and the temperature controller regulates a valve in the cooling stream by-passing (part of) the reactor. The pressure in the reactor is controlled by a pressure controller that regulates a valve in the product stream out of the reactor.

5.1.2 Distillation Columns

Feed streams
The flow-rates of the feed streams of distillation columns T7 and T21 are controlled by a pressure controller on the preceding reactor that regulates a valve in the reactor output stream and thus the column feed stream~~. The~~ feed flow-rates of columns T12 and T28 are set by the level controllers of column T7 and T21 respectively.

Condenser
It is important to be able to control the distillate streams of the columns rather well, for in many cases they contain the desired product. To do this, every column is equiped with a set of controllers in the condenser section. A pressure controller measures the pressure in the top stream leaving the column and signals a speedcontroller which, on its turn, regulates the speed of the aircooler fan(s). Furthermore a level controller measures the liquid level in the top accumulator and regulates a valve in the distillate stream. Finally a flow controller is placed in the reflux stream and regulates a valve in the same stream.

Stripping section and reboiler
To be able to control the bottom streams of the colums as well, the columns will also be equiped with a set of controllers in the stripping section and the reboiler section. The temperature is often used as an indication of composition. The temperature sensor should be located at the position in the column where the rate of change of temperature with change in composition of the key component

is big. The temperature controller will be placed somewhere in the stripping section where this is the case and it will be cascaded with a flow controller which regulates the flow-rate of the steam flow of the reboiler. Furthermore a level controller is placed at the bottom of the column and regulates a valve in the bottom product stream.

5.1.3 Heat Exchangers

The air cooled heat exchangers in the condenser sections of the columns are controlled by a cascade arrangement of a pressure controller and a speed controller. The pressure controller measures the pressure at the top of the column and acts as the master controller over the speed controller. The slave speed controller on its turn regulates the speed of the fans. The other air coolers are controlled by a cascade arrangement of a master temperature controller in the output stream and a speed controller.

5.1.4 Pumps

The rotary pumps used are all running at fixed speeds and are all equiped with the same standard control units. The output pressure is controlled by a by-pass control: the pressure is measured at the downstream side and the controller regulates a valve in the stream by-passing the pump. The output flow is controlled by a flow controller that regulates a valve in the output stream.

5.2 Safety Features

The process control equipment described above are installed to ensure stable operation of the plant. As said before it is very important to install extra control equipment such as alarms, safety trips and interlocks to alert operators of serious, and potentially hazardous, deviations in process conditions and thus to make the process as save as possible.

The equipment needing the most attention are the two reactors.They both will be equiped with an automatic trip system. This system contains the following basic components:

1. Temperature and pressure sensors that provide an output signal when a preset value is exceeded.
2. A system of electric relays to transfer the signal to an actuator.
3. An actuator to carry out the required action.

This action might for example be the closing of a valve in the catalyst feed of the first reactor or the PO feed of the second reactor. The closing of those streams will prohibit the reaction from occuring and hence control the temperature and pressure of the system.

Also the columns need extra attention. Additional temperature indicating or recording points will be included up the columns for monitoring column performance and for trouble shooting.

6. Safety, Health and Environment

In the next sections a short evaluation will be given about the safety, health and environmental (SHE) risks considering the process. Finally, a short Hazard and Operability (HAZOP) analysis will be presented in order to select the critical unit operation(s).

6.1 Safety, Health and Environmental Aspects.

The process comprises two hazardous substances. Both methanol and propylene oxide are toxic and very flammable substances. Therefore, it is important that those feed streams are handled with care. Spills of one of the substances, especially PO, is very dangerous due to the fact of (very) low lower explosion limits in air. Moreover, PO reacts readily and heavily with any agent containing active hydrogen atoms.

In general, the following safety measures should be considered. At first, all piping and instrumentation containing one of both substances should be checked regularly for leakage. Secondly, in case of sudden pressure increase, pressure relief valves are installed (for example in the reactor). The gaseous and flammable effluents are led to a flare. Finally, all electrical equipment, instrumentation and piping should be grounded electrically to prevent any build-up of static charges in the system. Only a spark is needed to initiate a major blow-out.

Fire protection is clearly needed. In case of methanol fire a complication occurs. Methanol flames are practically invisible in daylight. Thereby, water is not a suitable fire-extinguishing agent, because water dissolves in methanol. Protein-based alcohol-resistant foams are suitable and recommended for this job.

In case of propylene oxide fire, leakage or spills, water can be used. It is important to spray copious amounts of water to reduce the extent of vapour in the air (lower explosion limit is 1.9 %). Considering the environmental aspects of both substances it is necessary to prevent running-off of diluted PO or methanol to the sewer system. Containment walls should be built.

The hazardous nature of these substances leads to the conclusion that thoroughly trained personnel should be employed.

6.2 Waste Treatment

The waste stream leaving the process contains mainly higher propylene glycol ethers like MDP and MTP and catalyst. The catalyst is present as Na^+. The presence of catalyst in this stream makes disposal of this waste stream to some incineration unit necessary. In designing such a unit the formation of any toxic product should be prevented. If needed scrubber or stripping sections can be applied to clean off-gases.

Some measures, like ion exchanging, could be considered to recover Na^+. The resulting mixture of approximately equal amounts of MDP and MTP could be used as braking fluid. Recovered Na^+ and methanol can be mixed to recover catalyst.

6.3 HAZOP-analysis

The structure of the process indicates clearly that the first and section reaction section resemble each other strongly. Therefore, in the following HAZOP-analysis only the MP-2 reactor and the methanol recycle column are taken into account. The results for these units can be translated easily to other units.

As the HAZOP-analysis will show, critical units in the process are the reactors. Especially, the first reactor, having great amounts of both volatile methanol and propylene oxide, makes stable operation difficult. Temperature is a critical constant. If reactor inlet temperature is too high, unacceptable pressure build-up due to rapid reaction rates can lead to blow-out. As a result, temperature and pressure are considered as critical constants implying for example high level alarm systems.

The HAZOP-analysis for the MP-2 reactor is presented in Table 6.1 whereas the HAZOP-analysis for the methanol recycle column is presented in Table 6.2.

HAZOP-analysis for MP-2 reactor

Guide Word	Deviation	Possible Causes	Consequences	Action required
Not, No	No reactant flow	a. Pump failure	Loss of feed to reactor, possible rise in temperature and thus pressure due to loss of heat capacity	1.PC on reactor 2.Back-up pump
		b. Line blockage c. Leak !	As for a.	3. FC in piping before and after reactor
More	More flow	c. Increase MeOH feed stream	Total PO conversion not reached More MP produced Flatter temperature profile in reactor	4. FC in MeOH stream
		d. Increase PO feed stream	Heat production rate in reactor increases, thus temperature and pressure; possibility of run-away Selectivity towards MDP increases	5. FC in PO stream 6. High flow alarm for PO stream High T alar
		e. Increase cat feed stream	Reaction rates accelerated; max. temperature reached in reactor higher and thus pressure higher	7. FC in cat stream 8. High flow alarm for cat stream
		f. Increase of recycle flow	More cooling capacity; flatter temperature profile in reactor	9. FC in recycle stream
	More T	g. Inlet T higher	Reaction rates accelerated; max. temperature reached in reactor higher and thus pressure higher	10. TC in reactor inlet

Guide Word	**Deviation**	**Possible Causes**	**Consequences**	**Action required**
More	More T	h. Fouling of heat transfer area	Heat transfer decreases, reaction mixture temperature increases, accelerating rates and thus heat production	11. TC in reactor; tube-side as well as shell-side 12. Cleaning reactor tubes if necessary
		i. PO feed stream increases	As for d.	As for 5. and 6.
		j. Cat feed stream increases	As for e.	As for 7. and 8.
	More P	k. Max temperature reached in reactor higher	Pressure increase, due to temperature rise, giving way to reactor failure. Back flow out of reactor	As for 1. and 2. 13. One way valve in reactor entrance
		l. Pump rises pressure too much	Pressure increase leads to higher reactor inlet temperature and thus accelerated reaction rates, resulting in extra pressure increase due to reaction.	14. PC on pump
		m.Line blockage off-stream	As for k., except for the result of temperature increase	As for 1., 3., and 13.
Less	Less flow	n. MeOH feed stream decreases	Product distribution changes (more MDP) Cooling capacity decreases thus temperature and pressure higher in reactor.	As for 3.
		o. PO feed stream decreases	Production rate decreases; depending on the amount of feed stream decrease, temperature in reactor will increase or decrease.	As for 3. and 6.
		p. Cat feed stream decreases	Less conversion Temperature decrease in reactor	As for 3.
		q. Leakage of valves or flanges	As for n., o. and p. Emission to environment	As for 3.: FC in piping before and after reactor 15. Regular inspection
		r. Recycle stream decreases	As for n.	As for 3.

Guide Word	Deviation	Possible Causes	Consequences	Action required
	Less T	s. Feed stream is not preheated enough	Reaction will not really start, total conversion is not reached	As for 10.
		t. MeOH feed stream or recycle stream increased	As for c. and f.	As for 4. and 9.
	Less P	u. Leaking flanges	Emission to the environment	As for r.
		v. Pump failure	As for a.	As for 1.

Table 6.1: HAZOP-analysis for MP-2 reactor

HAZOP analysis for methanol recycle column

Guide Word	Deviation	Possible Causes	Consequences	Action required
Not, No	No feed flow	a. Line blockage	No feed flow to downstream units. No recycle/product streams	1.Regular maintenance
		b. Line fracture	As for a.	2.Regular maintenance and inspection
		c. Relieve valve failure	As for a.	As for 1.
More	More P	f. Failure of pressure relieve valve	Poor separation (more light key over bottom)	3.Install PC over pressure relieve valve
	More T	g. More heat formed in reactor	Poor separation (more heavy key over top)	4.Bigger reflux ratio (R/D)
Less	Less feed flow	h. Line blockage	Less feed flow to downstream units. Less recycle/product streams	As for 1.
		i. Line fracture	As for h.	As for 2.
		j. Failure of pressure relieve valve	As for h.	As for 1.
	Less T	k. Less heat formed in reactor	As for f.	5.Higher reboiler duty

Table 6.2: HAZOP-analysis for the methanol recycle distillation columns

7. Project Economics

In this chapter a preliminary cost estimation of the project at the flow-sheet stage is made as well as the project's economic evaluation. All the equations and values of the estimates used in this chapter can be found in Coulson and Richardson's [6]. The cost of the project can be divided into the total investment cost and the operating cost. The total investment cost is calculated with the use of a so called factorial method. Such a method is based on an estimate of the purchase cost of the major equipment items required for the process. The other costs are estimated as factors of the equipment costs. The operating costs, the costs of producing the product, can be estimated from the flow-sheet, the capital cost estimate and the operating labour estimate.

7.1 Total Investment Cost

The total investment cost ~~is comprised of~~ the fixed capital and the working capital. As said before the fixed capital can be calculated with the use of the Lang factorial method and the purchase cost of the major equipment items required for the process. The working capital is taken as a factor of the fixed capital.

7.1.1 Estimation of Purchased Equipment Costs

The estimation of the purchased equipment costs forms the basis of the Lang method and must be determined as accurately as possible. The prices for the equipment, except for the air coolers, are derived from the DACE-prijzenboekje [29]. The depicted data are prices for september 1995. The method usually used to update historical cost data makes use of published cost indices. These relate present costs to past costs, and are based on data for labour, material and energy costs published in government statistical digests and therefore account for inflation. The correction is performed using the following equation:

$$Cost\ (1997) = Cost\ (\underset{x}{19..}) \cdot \frac{Cost\ index\ 1997}{Cost\ index\ 19.._{x}} \qquad x = 1995 \qquad (7.1)$$

The cost index numbers used are taken from the DACE-prijzenboekje as well and are shown in Table 7.1. The year 1985 is taken as the reference year (index 100). The index number for 1997 is extrapolated from the historic values.

Year	1985	1987	1995	1997
index number	100	102	116	119

Table 7.1: Index numbers

The calculated equipment costs are given in Table 7.2 on the next page. A more detailed calculation is given in Appendix H.1.

Equipment	Equip. n°	Cost (kfl)	Equipment	Equip. n°	Cost (kfl)
reactor	R 5	287.82	air cooler	H 33	11.03
reactor	R 19	110.92	condenser	H 9	107.57
tower	T 7	354.76	condenser	H 10	72.14
tower	T 12	904.15	condenser	H 23	20.14
tower	T 21	194.88	condenser	H 30	14.10
tower	T 28	44.79	reboiler	H 8	180.55
air cooler	H 18	21.65	reboiler	H 13	324.17
air cooler	H 26	34.28	reboiler	H 22	26.67
air cooler	H 34	20.45	reboiler	H 29	30.26
Purchased equipment costs:					**3,278**

Table 7.2: Purchased equipment costs

7.1.2 Fixed Capital Costs

The fixed capital cost of the project is given as a function of the total purchase equipment cost, as follows:

$$C_f = f_L \cdot PCE \qquad (7.2)$$

where: C_f = fixed capital cost
PCE = the total delivered cost of all the major equipment items
f_L = the 'Lang factor'

The 'Lang factor' depends on the type of process being used. For predominantly fluids processing plants, like this process, a value of 4.7 can be taken as a rough estimate [6].
To make a more accurate estimation, the cost factors compounded into the 'Lang factor' are considered individually. These fixed capital costs can be divided into direct and indirect costs.

The direct-cost items that are usually incurred in the construction of a plant, in addition to the cost equipment are:

- Equipment erection, including foundations and minor structural work.
- Piping, including insulation and painting.
- Electrical power and lighting.
- Instruments, local and control room.
- Process, buildings and structures.
- Site and site preparation.
- Storage, raw materials and finished product.
- Utilities (Services), provision of plant for steam, water, air, firefighting services (if not costed seperately).

- Ancillary buildings, offices, laboratory buildings, workshops.

In this design, the last three factors are not taken into account for the calculation of the direct cost because they are either outside the battery limit or are already present at the site.

In addition to the direct cost of the purchase and installation of equipment, the capital cost of a project will include the indirect costs listed below.

- Design and engineering costs, which cover the cost of design and the cost of 'engineering' the plant: purchasing, procurement and construction supervision.
- Contractor's fees.
- Contingency allowance.

The contribution of each of these items to the total capital cost is calculated by multiplying the total purchased cost of equipment (PCE) by an appropriate factor. Typical factors, based on historical cost data of other fluids processing plants, are given in Table 7.3.

Item	Factor n°	Factor value
Equipment erection	f_1	0.40
Piping	f_2	0.70
Instrumentation	f_3	0.20
Electrical	f_4	0.10
Buildings, process	f_5	0.15
Site development	f_6	0.05
Total direct-cost items	1+ fact	**1.60**
Design and engineering	f_7	0.30
Contractor's fees	f_8	0.05
Contingency allowance	f_9	0.10
Total indirect-cost items	1+fact	**0.45**

Table 7.3: Typical factors for estimation of project fixed capital cost

The total physical plant cost (PPC) is calculated as follows:

$$PPC = PCE(1 + f_1 + \ldots + f_6) = PCE(1 + 1.60) = 2.60PCE \qquad (7.3)$$

The fixed capital cost can now be calculated, using the following formula.

$$C_f = PPC \cdot (1 + f_7 + f_8 + f_9) = 2.60\,PCE \cdot 1.45 = \underline{\underline{3.77}}\,PCE \qquad (7.4)$$

7.1.3 Working Capital

Working capital is the additional money required over and above the fixed capital, to start up the plant and operate it to the point when income is earned. It includes the cost of:

- Start-up: includes process modifications, start-up labour and loss in production.
- Initial catalyst charges.
- Raw materials and intermediates in the process.
- Finished product inventories.
- Funds to cover outstanding accounts from customers.

As said before, when applying the Lang method, the working capital is estimated as a percentage of the fixed capital costs. According to C&R, the estimate range is 10-20% of the fixed capital costs. In this case 15% is taken as the estimate percentage. High!

Now, the total investment costs can be calculated, adding the fixed and working capital.

Fixed capital cost (kfl)	12,358
Working capital (kfl)	1,854
Total investment required for the project (kfl):	**14,212**

low!

Table 7.4: Total investment costs

7.2 Operating Costs

An estimate of the operating costs, the cost of producing the product(s), is needed to judge the viability of the project. The operating costs can be calculated in a way simular to the calculation of the total investment cost. They are are divided into direct and indirect costs and the direct costs are subdivided into fixed costs and variable costs. These direct and indirect costs be calculated from the flow-sheet, the capital cost estimate and the operating labour cost estimate. Simply adding of the direct and indirect costs gives the total annual operating cost.

An overview of all the costs making up the operating costs is given in the following sections.

7.2.1 Direct Operating Costs

As mentioned above, the direct operating costs include variable and fixed costs. Costs which are dependent on the amount of product produced belong to the variable costs.

7.2.1.1 Variable Costs

The variable costs include:

- Raw materials.
- Miscellaneous operating materials.
- Utilities (Services).

Raw materials.
These are the major materials required to manufacture the products. The quantities can be obtained from the flow-sheet and multiplied by the price to get the annual costs.

Raw materials	**Consumption (kt/a)**	**Price (kfl/kt)**	**Costs (kfl/a)**
MeOH	33.031	342	11,297
PO	61.967	1,938	120,092
kat	1.278	950	1,214
Total raw material cost			**132,603**

Table 7.5: Raw material costs per year.

Miscellaneous materials (plant supplies).
Under this heading are included all the miscellaneous materials required to operate the plant that are not covered under the headings raw materials or maintenance materials. Such as, safety clothing, instrument charts and gaskets. As a rough guide, the cost of miscellanous materials can be taken as 10 % of the maintenance cost.

Utilities.
The annual cost of utilities used, like steam and power, can be calculated from the flow-sheet and the given prices.

Utilities	**Consumed (kt/a)**	**Price (kfl/kt)**	**Costs (kfl/a)**
Low pressure steam	79.23	20	1,585
Middle pressure steam	139.41	27	3,764
Total steam cost			5,349

Table 7.6: Steam costs per year.

	Consumed MW	**Consumed MJ/a**	**Consumed kWh/a**	**Price kfl/kWh**	**Costs kfl/a**
Electricity	0.156	4,717,440	1,310,400	8.5e-5	111.38

Table 7.7: Electricity costs per year.

7.2.1.2 Fixed Costs

Fixed costs are costs that do not vary with the production rate. They include:

- Maintenance (labour and materials).
- Operating labour.
- Laboratory costs.
- Supervision.
- Plant overheads.
- Capital charges.
- Local taxes.
- Insurance.
- Licence fees and royalty payments.

Maintenance.
Includes the cost of maintenance labour and materials needed for the maintenance of the plant. The annual maintenance costs for chemical plants are high, typically 5-15% of the fixed capital costs. As a rough estimate the annual maintenance cost is taken as 10% of the fixed capital cost.

Operating labour.
This is the manpower needed which is directly involved with running the process. Because of the small size of the plant, only two men will be needed to operate the plant. To operate three shifts a day, at least five shift crews will be needed. This means at least 10 men are needed as operating labour. The cost of each man is estimated as being fl 118,000 a year. These costs include shift allowance, a thirteenth month, allowance for holidays, national insurance, total pension contributions etc.

Supervision.
Assumed are two operating managers for the whole plant. The cost of each manager is estimated as fl 127,000 a year. These costs include the same allowances as for operating labour except shift allowance.

Laboratory costs.
These are the annual cost of the laboratory analyses required for process monitoring and quality control. As a rough estimate the costs are taken as 25% of the operating labour cost.

Plant overheads.
Included under this heading are all the general costs associated with operating the plant not included under the other headings; such as general management, plant security, medical and canteen services. A typical range of these costs is 50 to 100% of the operating labour costs; depending on the size of the plant and whether the plant is built on a new site, or an extension of an existing site. Since the plant is small with little personnel working on it and is built on a existing site, the lower limit of the typical range is taken as the estimate: 50% of the labour costs.

Capital charges.

The investment required for the project is recovered as a charge on the project. Rather than to consider the cost of capital as depreciation or interest, it is easier to take the cost as a straight, unspecified, capital charge on the operating cost. Here, 6.67 % of the fixed capital (annually) is taken as the estimate of the capital charge.

Local taxes.

A typical estimation of the taxes that have to be paid is 2% of the fixed capital costs.

Insurance.

Contains the annual insurance premium paid to the insurers for the site and plant insurance. A typical value is 1% of the fixed capital.

Royalties and licence fees.

The proces has been developed exclusively by the operating company therefore no royalties and licence fees have to be paid.

7.2.2 Indirect Operating Costs

The indirect operating costs are costs that arise from the fact that the site will have to pay a share of the company's general operating expenses. These include:

- Sales expense.
- General overheads.
- Research and development costs.
- Reserves.

The costs of the individual indirect operating costs vary from company to company. As a range of estimate 20 to 30% of the direct operating costs is usually taken. For this methoxy propanol plant 20% of the direct operating costs is used.

Table 7.8 below gives an overview of the operating costs discussed above.

Item	Typical value	Cost (kfl/a)
Raw materials	see Table 7.5	132,603
Miscellaneous operating	10 % of the maintenance cost	123.60
Utilities (Services)	see Table 7.6 and 7.7	5,460.38
Total variable costs (A)		**138,186.98**
Maintenance	10% of fixed capital	1,236
Operating labour	-	1,180
Laboratory costs	25% of labour costs	295.00
Supervision	-	254.00
Plant overheads	50% of ~~labour costs~~	590.00
Capital charges	6.67% of fixed capital	824.41
Local taxes	2% of fixed capital	247.00
Insurance	1% of fixed capital	123.50
Total fixed costs (B)		**4,749.91**
Total direct production cost (A+B)		**142,936.89**
Indirect operating costs	20% of A+B	28,587.37
Total indirect operating costs (C)		**28,587.37**
Total annual operating costs (A+B+C)		**171,524.26**

Table 7.8: Summary of production costs.

7.3 Economic Evaluation of the Project

As the purpose of investing money in a chemical plant is to earn money, some means of comparing the economic performance of the project is needed. A few techniques of economic evaluation, the criteria used to judge the economic performance of the plant and the results of the calculations are outlined in this section. The criteria can be divided into two groups: static criteria and dynamic criteria. The former do not account for the time value of money whereas the latter do. Also the lifetime of the project does not always play a role in static criteria whereas it does in dynamic criteria. Examples of static criteria are pay-back time (PBT) and rate of return (ROR). Examples, given here, of dynamic criteria are the net present worth (NPW) and total net present worth (TNPW) of the project and the discounted cash-flow rate of return (DCFRR). There is no one best criterion on which to judge the investment opportunity. The criterion used depends on the kind of project and the company's preference. The calculation and some tables of the different criteria can be found in Appendix H.2.

In the sections above only the costs of the project were discussed and not the incomes. The earnings of the project come from the sales of the products MP-2 and MDP. Table 7.10 shows the sales figures of the plant.

Product	Sales quantity (kt/a)	Price (kfl/kt)	Income (kfl/a)
MP-2	85.024	1824	155,084
MDP	15.005	1824	27,369
Total			**182,4[illegible]3**

Table 7.10: Sales figures for the sale of MP-2 and MDP

7.3.1 Cash-flow Diagram.

The net cash flow at any time is the difference between the earnings and expenditure which, on their turn, are based on the estimates of sales volumes, sales prices, investment and operating costs that have been made for the project. The cash-flow diagram below shows the forecast cumulative net cash flow over the life time of the project. The diagram gives a clear picture of the resources required for the project and the timing of the earnings. The designing of the plant is assumed to last 1 year, the actual building (start-up included) 2 years.

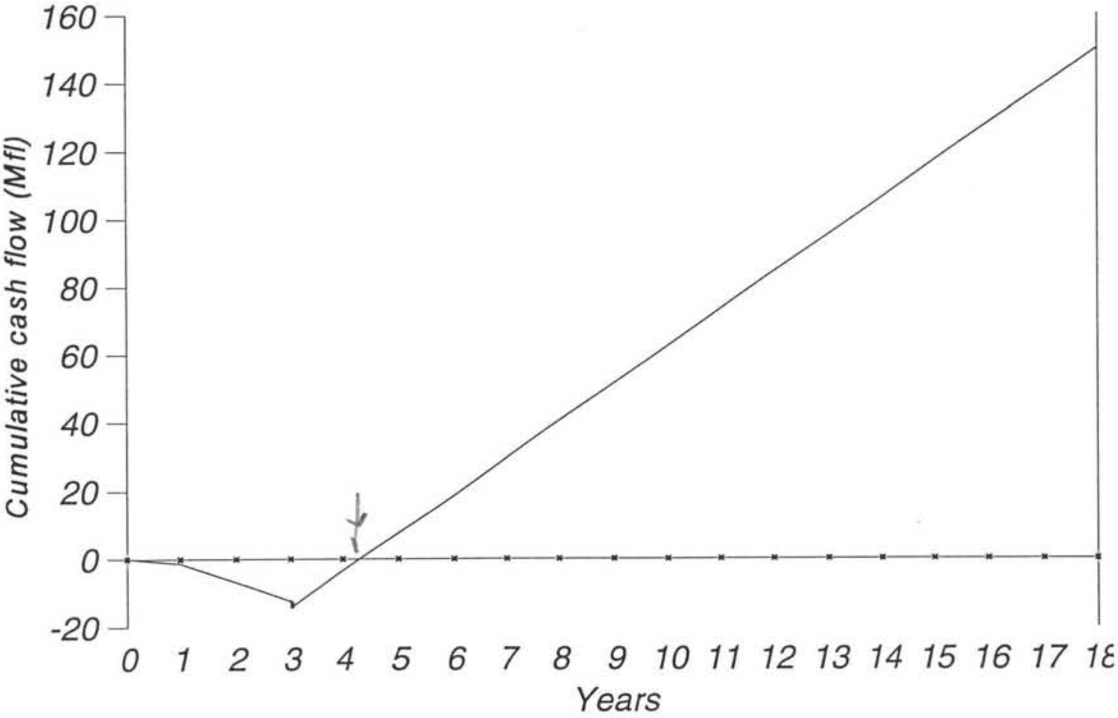


Figure 7.1: Cash-flow diagram

7.3.2 Pay-back Time.

The pay-back time is defined as the time required after the start of the project to pay off the initial investment from income. Pay-back time as a criterion of investment performance does not, by this definition, consider the performance of the project after the pay-back time.
The pay-back time can be calculated or read from the cash-flow diagram. The pay-back time for this methoxypropanol plant is 4 years and 4 months.

7.3.3 Rate of Return.

Cash-flow figures do not show how well the capital invested is being used. Some way of measuring the performance of the capital invested is needed. The rate of return (ROR) is the ratio of annual profit to investment and is a simple index of the performance of the money invested. The simplest method is to base the ROR on the average income over the life of the project and the original investment. This method takes into account the fact that the annual profit will not be constant over the life of the project -although that is not shown in the cash-flow diagram. The ROR can be calculated using formula 7.5.

$$ROR = \frac{F - C}{C \cdot G} \cdot 100\% \qquad (7.5)$$

where: F-C = cumulative income (*f*)
C = investment (*f*)
G = life of the project (*f*)

The ROR for this project is 63.56%.

7.3.4 Net Present Worth (NPW) and Total Net Present Worth (TNPW).

Figure 7.1 shows the net cash flow at its value in the year in which it occurs. So the values on the y-axis show the "future worth" of the project: the cumulative "net future worth", NFW. A way to account for the time value of money is to calculate the net present worth (NPW) of cash flow. The NPW can be calculated by using formula 7.6 below.

$$NPW = \frac{NFW \ in \ year \ n}{(1 + r)^n} \qquad (7.6)$$

where: r = discount rate (interest rate) (-)

The discount rate is taken to be 0.16.

The total net present worth (TNPW) can be calculated as follows:

$$TNPW = \sum_{n=1}^{n=t} \frac{NFW}{(1+r)^n} \tag{7.7}$$

The TNPW will be less than the total NFW, and reflects the time value of money and the patterns of earnings over the life of the project.

To get an easy and quick overview, the results are shown in Figure 7.2.

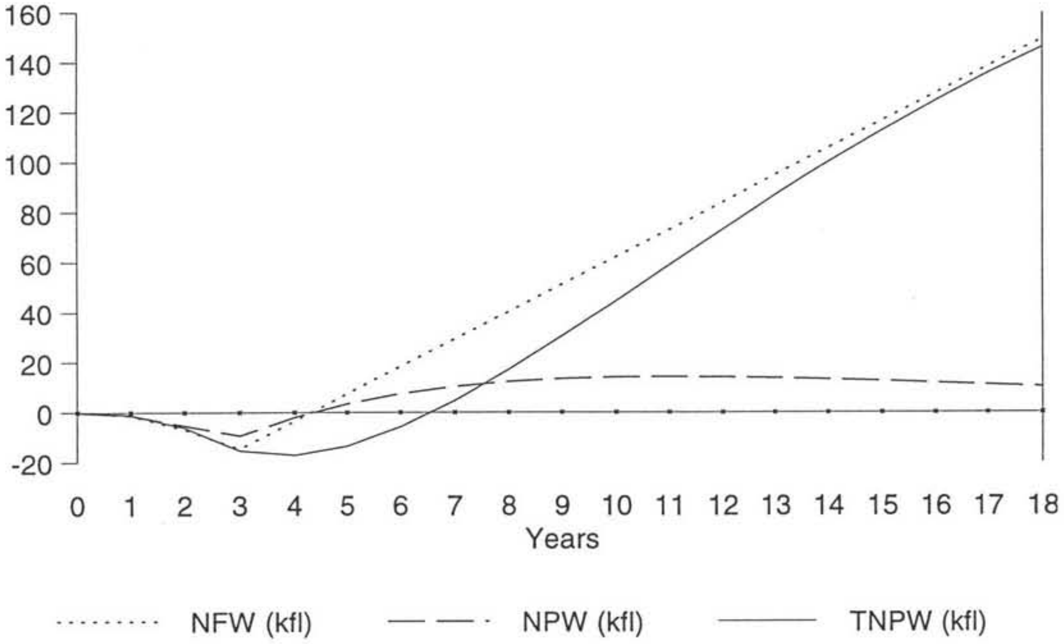


Figure 7.2: Results of the dynamic criteria calculations

7.3.5 Discounted Cash-flow Rate of Return (DCFRR).

The discounted cash-flow rate of return (DCFRR) is the maximum interest rate that the project could pay and still break even by the end of the project life. The value is found by trial-and-error calculations using formula 7.8.

$$\sum_{n=1}^{n=t} \frac{NFW}{(1+r')^n} = 0 \tag{7.8}$$

Where: r' = discounted cash-flow rate of return (-)
The discounted cash-flow rate of return for this methoxy propanol plant is 0.565. 56.5%

The investment criteria discussed in this section are set out in Table 7.11, which shows the main advantage and disadvantage of each criterion.

Criterion	Advantage	Disadvantage
PBT	Shows how soon investment is recovered	No information on later years
ROR	Measures performance of capital	Takes no account for time value of money. Depends on definition of income and investment
NFW Net fut worth	Simple Shows timing of investment and income	Takes no account for time value of money
NPW Net Pres worth	As for NFW but accounts for timing of cash flows	Depends on discount rate used
DCFRR	Measures performance of capital accounting for time value of money	No indication of the resources needed

Table 7.11: Investment criteria and their advantages and disadvantages

8. Conclusions and Recommendations

The objective of the assignment, to design a plant for the production of 85,000 t/a MP-2 and 15,000 t/a MDP with respective purities of at least 99.9 %w and 99.0 %w, has been met.

The production of MP-2 is 85,024 t/a. It has a purity of 99.92 %w, containing 0.051 %w MP-1 and 0.0087 %w MeOH. The production of MDP is 15,005 t/a. Its purity is 99.12 %w, containing 0.055 %w MP-1.

In absence of purges, the conversion of MeOH and PO is 100 %. Only minor losses to side products occur. The catalyst used in the process is the homogeneous ~~base~~ sodiummethylate ($NaOCH_3$).

The waste stream is 2,958 t/a, resulting in a waste percentage of 2.87 %. Due to the presence of Na^+, this stream is ready for waste treatment. However, some recovery measures like ion-exchange could be considered. The remaining mixture of MDP and MTP, free from Na^+, can be used as brake fluid whereas the removed Na^+, after regeneration, can be recycled to the first reactor section. This implies a continuous catalyst regeneration cycle.

The process structure is simple. The two-reactor configuration leads to operation optimised for the main reaction taking place in the respective reaction sections. Another feature of this configuration is the built-in flexibilitiy. If market demands would change, production rates of MP-2 and MDP can be adjusted to meet these demands.

The heat integration in the process is done by use of heat exchange in both reactors. The heat of reaction is utilised to preheat the feed streams before entering the reactor. In effect, the reactor can be looked upon as a shell and tube heat exchanger with reaction taking place within the tubes. Further, only coolers are applied in the process. Due to the absence of cooling water, air is used to meet cooling requirements. All coolers are designed as air-fan coolers. Therefore, the temperature of the product streams can not be lower than 60°C.

Energy and power integration in the distillation columns needs further investigation. It is likely that energy savings are attainable when integrating the columns.

The safety of this process is a major concern. Beside the hazardous and readily flammable substances PO and MeOH, reactors are considered to be critical units. Controlling temperature and pressure in these units is very important to be able to maintain stable and safe operation of the process.

The process as designed is a profitable plant, making 10.9 million guilders a year. This leads to a pay-out time of 4 years and 4 months. Assumed that the designing and construction of the plant takes 3 years, it can be concluded that the investment is being recovered after 1 year and 4 months after the start-up of the plant. These satisfying figures present an estimate of the economics of the process. They lie within the so called 30% certainty area and should be considered as a first raw estimate.

9. References

1. Benson, S.W., *Thermochemical Kinetics,* Wiley Interscience, 2nd ed., New York (1976).

2. Bibo, B.H., Lemkowitz, S.M., *Chemical Risk Management*, lecture notes, TU Delft (1994).

3. Bleek, C.M. van den, Gerritsen, A.W. and Schouten, J.C., *Reactorkunde I*, lecture notes, TU Delft (1994).

4. Brown, R., *Design of Air-cooled Heat Exchangers: a Procedure for Preliminary Estimates*, Chem. Eng., 85 (March 27), New York (1978).

5. *Chemiekaarten*, 12th ed., Samsom H.D. Tjeenk Willink, Alphen aan de Rijn (1996).

6. Coulson, J.M. and Richardson, J.F., *Chemical Engineering, Volume 6*, 2nd ed., Pergamon Press, Oxford (1993).

7. Coulson, J.M. and Richardson, J.F., *Chemical Engineering, Volume 1,* 4th ed., Pergamon Press, Oxford (1990).

8. De Loos, Th. W., Van der Kooi, H.J., *Toegepaste thermodynamica voor ontwerpers*, lecture notes, TU Delft.

9. De Graauw, J., Paijens, A., *Pompen en Compressoren*, lecture notes, TU Delft (1995).

10. Dean, J.A., *Lange's Handbook of Chemistry,* 14th ed., McGraw-Hill, New York (1992).

11. Douglas, J.M., *Conceptual Design of Chemical Processes*, McGraw-Hill, New York (1988).

12. *Economic Indicators,* Chem. Eng., vol.103 (March), New York (1996).

13. *Economic Indicators,* Chem. Eng., vol .104 (November), New York (1997).

14. Fogler, H.S., *Elements Chemical Reaction Engineering,* Prentice-Hall, 2nd ed., Englewood Cliffs (1992).

15. Garret, D.E., *Chemical Engineering Economics,* Van Nostrund Reinhold, New York (1989).

16. Glass, J., *Specifying and rating fans,* Chem. Eng., vol. 85 (March 27), New York (1978).

17. Janssen, L.P.B.M., Warmoeskerken, M.M.C.G., *Transport Phenomena Data Companion*, Delftse Uitgevers Maatschappij, Delft (1991).

18. Kern, D.Q., *Process heat transfer,* 24th ed., McGraw-Hill, Singapore (1988).

19. Kirk-Othmer, *Encyclopedia of Chemical Technology,* 4th ed., Vol.A20, Wiley Interscience, New York (1997).

20. Levenspiel, O., *Chemical Reaction Engineering,* 2nd ed., Wiley Interscience, New York (1972).

21. Lide, D.R. et al., *Handbook of Chemistry and Physics,* 76th ed., CRC Press, Boca Raton (1995).

22. Perry, R.H., Green, D.W., *Chemical Engineer's Handbook,* 70th ed., McGraw-Hill, New York (1997).

23. Reid, R.C., Prausnitz, J.M., Poling, B.E., *The properties of gases and liquids,* 4th ed. McGraw-Hill, New York (1992).

24. Richardson, J.F. and Peacock, D.G., *Chemical Engineering, Volume 3,* 3th ed., Pergamon Press, Oxford (1994).

25. Schnurpfeil, D.et al, *Verfahren zur gleichzetigen Herstellung von isomerenreinem Propylenglycol-mono-methylether und Dipropylenglycol-mono-methylether,* DE patent nr 19525067 A1 (1997).

26. Smith, J.M. and Van Ness, H.C., *An Introduction to Chemical Engineering Thermodynamics*, 4th ed., McGraw-Hill, New York (1987).

27. Stephanopoulos, G., *Chemical Process Control: An introduction to theory and practice*, Prentice Hall, Englewood Cliffs (1984).

28. Ullmann, F., Gerhartz, W., *Ullmann's Encyclopedia of Industrial Chemistry,* 5th ed., Vol. A22, Verlag Chemie, Weinheim (1985).

29. Webci en Wubo, DACE-Prijzenboekje: Kostgegevens t.b.v. ramingen, Dutch Association of Cost Engineers, 18th ed., Weevers, Vorden (1995).

30. Wesseling, J.A., Kleizen, H.H., *Scheidingsprocessen*, 2nd ed., Delftse Uitgevers Maatschappij, Delft (1992).

10. List of symbols

Chapter 4.1: Reactor design

$A_{cr,t}$	cross flow area tube	m^2
$A_{cr,s}$	cross flow area shell	m^2
C_i	concentration of component i	mol/m^3
$C_{p,i}$	heat capacity of componet i	J/mol°C
D_b	bundle diameter	m
d_e	equivalent diameter	m
d_i	inside tube diameter	m
d_o	outside tube diameter	m
D_s	shell diameter	m
h_i	inside fluid film coefficient	$W/m^2{}^\circ C$
h_{id}	inside dirt coefficient	$W/m^2{}^\circ C$
h_o	outside fluid film coefficient	$W/m^2{}^\circ C$
h_{od}	outside dirt coefficient	$W/m^2{}^\circ C$
j_f	friction factor	-
j_H	heat transfer factor	-
k	thermal conductivity	W/m°C
k_w	thermal conductivity of tube wall material	W/m°C
L	tube length	m
l_B	baffle spacing	m
N_p	number of tube passes	-
N_t	number of tubes	-
Pr	Prandtl number	-
Q	heat duty	W
Re	Reynolds number	-
r_i	production rate of component i	mol/m^3s
T	reactor temperature	°C
T_{feed}	feed temperature	°C
U	heat transfer coefficient	$W/m^2{}^\circ C$
u_s	shell-side velocity	m/s
u_t	tube-side velocity	m/s
V	reactor volume	m^3
ΔH_f	heat of formation	J/mol
ΔH_R	overall heat of reaction	J/mol
ΔP_s	shell-side pressure drop	Pa
ΔP_t	tube-side pressure drop	Pa
ΔT_m	mean temperature difference	°C
μ	viscosity	Pa·s
μ_w	viscosity of the wall	Pa·s
ν_i	stochiometric coefficient of component i	-
ρ	density	kg/m^3
τ	residence time	s
ϕ_v	volumetric flow	m^3/s

Chapter 4.2: Distillation columns

Column dimensions

A_a	active area	m^2
A_{col}	total column cross-sectional area	m^2
A_d	perforated area (including blanked areas)	m^2
A_d	downcomer cross-sectional area	m^2
A_h	hole area	m^2
A_{net}	net area for vapour-liquid disengagement	m^2
F_{LV}	liquid-vapour flow factor	-
d_{col}	column diameter	m
K_1	flooding velocity constant	m/s
u_f	flooding vapour velocity based on net area	m/s
ρ_l	liquid density	kg/m^3
ρ_v	vapour density	kg/m^3
σ	liquid surface tension	N/m
$\phi_{m,v}$	vapour mass flowrate	kg/s
$\phi_{m,l}$	liquid mass flowrate	kg/s

Plate dimensions

C_o	orifice coefficient	-
d_h	hole diameter	m
h_b	downcomer back-up	mm liquid
h_d	dry plate drop	mm liquid
h_{dc}	head loss in downcomer	mm liquid
h_{ow}	weir crest	mm liquid
h_r	residual head	mm liquid
h_t	total plate drop	mm liquid
h_w	weir height	mm
K_2	constant, depanding on clear liquid depth	$kg^{1/2} / m^{5/2}s$
l_w	weir length	m
t_r	residence time	s
$u_{h,min}$	minimum vapour velocity through holes	m

Chapter 4.3: Heat exchangers

A	heat transfer area	m^2
C_p	specific heat	kJ/kg·°C
F_t	correction factor	-
Q	heat transferred per unit time	W
P	dimensionless temperature ratio	-
R	dimensionless temperature ratio	-
S	dimensionless temperature ratio	-
T_1	inlet shell-side fluid temperature	°C
t_1	inlet tube-side fluid temperature	°C
T_2	outlet shell-side fluid temperature	°C
t_2	outlet tube-side fluid temperature	°C
T_{in}	inlet temperature	°C
T_{out}	outlet temperature	°C
U	heat transfer coefficient	$W/m^2 \cdot °C$
ΔH_{vap}	heat of vaporization	kJ/kg
ΔT_{lm}	logarithmic mean temperature difference (LMTD)	°C
ΔT_m	mean temperature difference	°C
ϕ_m	mass flow	kg/s

Chapter 4.4: Pumps

ΔP	pressure differential across the pump	Pa
ϕ_v	volumetric flow rate	m^3/s
η_p	pump efficiency	% or -

Chapter 7: Economics

f_L	Lang factor	-
PCE	purchase cost of equipment	fl
C	total investment	fl
C_f	fixed capital cost	fl
DCFRR	discounted cash-flow rate of return	-
F	cumulative cash-flow at end of plant life	fl
G	life of the project	yrs
n	year of project from start	yrs
NFW	net future worth	fl
NPW	net present worth	fl
PBT	pay-back time	yrs
PPC	physical plant cost	fl
r	discount rate	-
r'	discounted cash-flow rate of return	-
ROR	rate of return	-
TNPW	total net present worth	fl

11. Appendices

A. Process flow diagram

B1. Mass and Heat Balance
B2. List of Stream Compositons

C1. Substances in the Process
C2. Reaction Mechanism

D. Kinetics

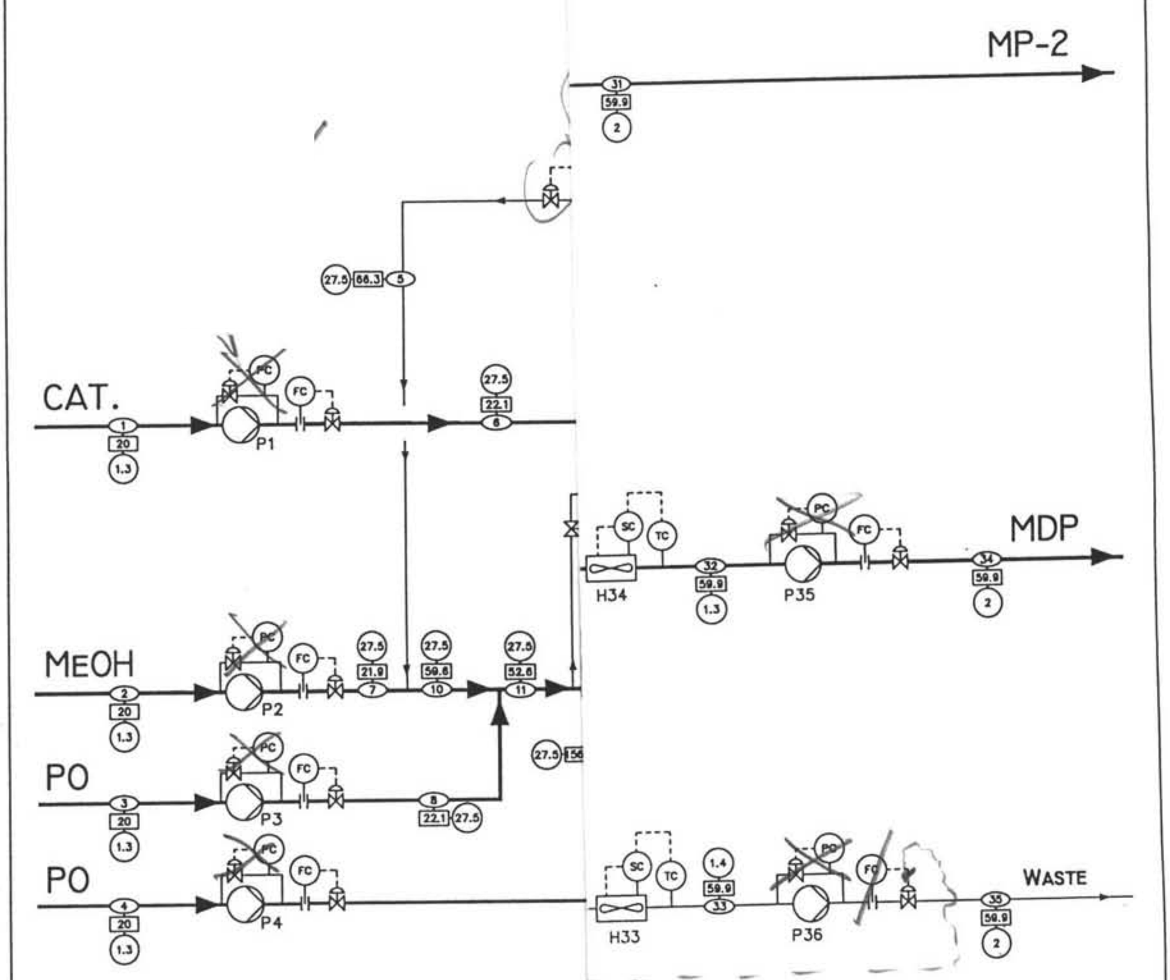
E1.1 Mass and Energy Balances Reactors
E1.2 Calculation of Stoichiometric Coefficients and Overall Heat of Reaction
E1.3 Reactor Design
E2.1 Overview Distillation Column Calculations
E2.2 Distillation Column Calculations
E3. Heat Exchangers Calculations
E4. List of Utilities

F1. Specification Forms Distillation Columns
F2. Specification Forms Heat Exchangers
F3. Specification Forms Pumps

G1. Equipment List for Reactors and Distillation Columns
G2. Equipment List for Heat Exchangers
G3. Equipment List for Pumps

H1. Equipment Costs
H2. Economic Evaluation Criteria

APPENDIX A: PROCESS FLOW



P1	pump	H8	reboiler	H15	cond
P2	pump	H9	condenser	V16	top
P3	pump	V10	top accumulator	P17	pum
P4	pump	P11	pump	H18	air c
R5	reactor	T12	dist. column	R19	reac
P6	pump	H13	reboiler	P20	pum
T7	dist. column	P14	pump	T21	dist.

(MP-2)

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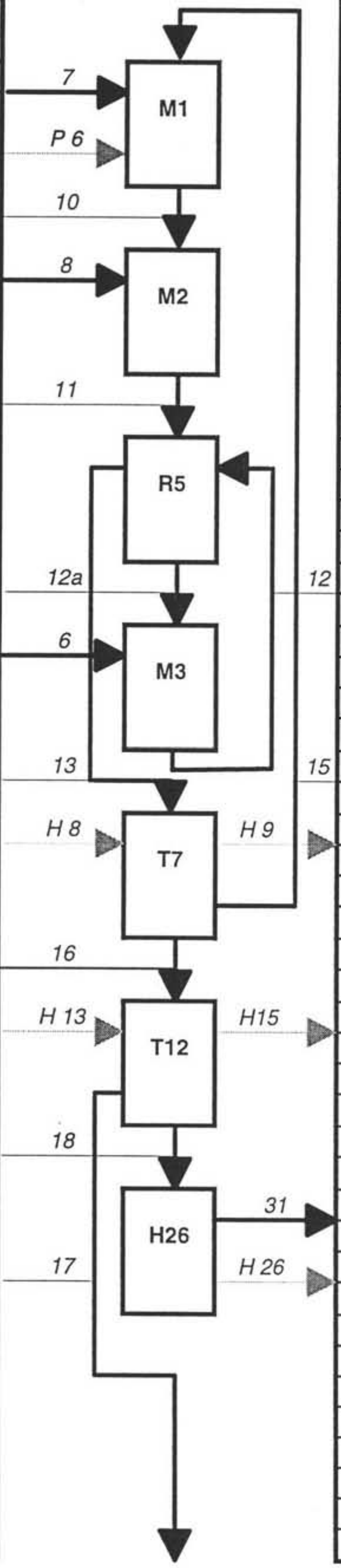
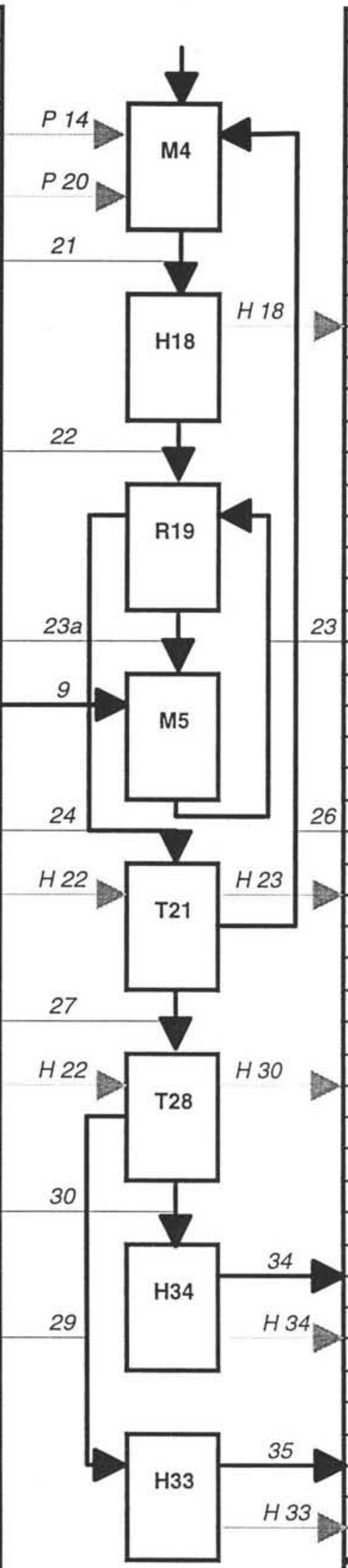
FVO 3206 January 1998

Appendix B1: Mass and Heat Balance



In M (kg/h)	In Q (MJ/h)	Forward M Q	Stream	Stream	Retour M Q	Out M (kg/h)	Out Q (MJ/h)
3932.2	-29515.2		7				
	105.9		P 6				
		24857.6 -183246.5	10				
7377.0	-15609.8		8				
		32234.6 -198856.2	11				
		32234.6 -188174.6	12a	12	32386.7 -189169.3		
152.1	-994.7		6				
		32386.7 -199888.5	13	15	20927.9 -153860.7		
	21260.0		H 8	H 9			28461.8
		11458.8 -53229.5	16				
	26087.3		H 13	H15			26039.0
		10121.9 -47647.7	18	31		10121.9	-49444.1
		1336.9 -5530.4	17	H 26			1796.4

Appendix B1: Mass and Heat Balance ctd.



In M (kg/h)	In Q (MJ/h)	Forward M	Forward Q	Stream	Unit	Stream	Retour M	Retour Q	Out M (kg/h)	Out Q (MJ/h)
	2.6			P 14	M4					
	10.4			P 20	M4					
		6534.2	-27540.9	21	H18					
					H18	H 18				828.9
		6534.2	-28369.8	22	R19					
		6534.2	-26499.8	23a	M5	23	7334.2	-28173.2		
800.0	-1673.4			9	M5					
		7334.2	-30044.7	24	T21	26	5197.3	-22023.5		
	470.0			H 22	T21	H 23				998.6
		2138.4	-8555.8	27	T28					
	662.1			H 22	T28	H 30				651.7
		1786.3	-7201.6	30	H34					
					H34	34			1786.3	-7822.8
					H34	H 34				621.2
		352.1	-1345.9	29	H33					
					H33	35			352.1	-1487.6
					H33	H 33				141.7
12261.3	805.2				**TOTAL**				12260.3	784.8

Appendix B2: List of stream compositions

Stream Number Name	1 Cat feed kg/h.	2 MeOH fd.	3 PO to R5	4 PO to R4	5 MeOH recycl.	6	7	8	9
Components									
MeOH	114	3928.3	0	0	20917.35	114	3928.3	0	0
PO	0	0	7377	800	6.78	0	0	7377	800
H2O	0.114	3.93	0	0	3.78	0.114	3.9283	0	0
MP-1	0	0	0	0	0	0	0	0	0
MP-2	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
MDP	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**
MTP	0	0	0	0	0	0	0	0	0
PG	0	0	0	0	0	0	0	0	0
NaOCH3	38	0	0	0	0	38	0	0	0
DPG	0	0	0	0	0	0	0	0	0
M4P	0	0	0	0	0	0	0	0	0
Mass flow (kg/h)	152.11	3932.23	7377.00	800.00	20927.91	152.11	3932.23	7377.00	800.00
Enthalpy (MJ/h)	-995.28	-29533.44	-15642.50	-1675.04	-153754.84	-994.69	-29515.16	-15609.77	-1673.42

Appendix B2: List of stream compositions

= 1+2+3

Stream Number	10	11	12	12A	13 R5 Effl.	14	15	Btms T7 16	17
Components									
MeOH	24843.76	24843.76	24957.76	24843.76	20918.23	20918.23	20917.35	0.88	0
PO	6.78	7383.78	7383.78	7383.78	6.78	6.78	6.78	0	0
H2O	7.01	7.09	7.2	7.09	6.14	6.14	3.78	2.36	0
MP-1	0	0	0	0	1068.27	1068.27	0	1068.27	1063.17
MP-2	**0**	**0**	**0**	**0**	**10214.28**	**10214.28**	**0**	**10214.27**	**100.7**
MDP	**0**	**0**	**0**	**0**	**129.65**	**129.65**	**0**	**129.65**	**129.65**
MTP	0	0	0	0	0.61	0.61	0	0.61	0.61
PG	0	0	0	0	4.14	4.14	0	4.14	4.14
NaOCH3	0	0	38	0	38	38	0	38	38
DPG	0	0	0	0	0.62	0.62	0	0.62	0.62
M4P	0	0	0	0	0	0	0	0	0
Mass flow (kg/h)	24857.55	32234.63	32386.74	32234.63	32386.72	32386.72	20927.91	11458.80	1336.89
Enthalpy (MJ/h)	-183246.45	-198856.22	-189169.25	-188174.56	-199888.55	-199888.48	-153860.70	-53229.48	-5530.36

Appendix B2: List of stream compositions

Stream Number	18	Btms T12 19	20 MP1 rec.	21	22	23	23A	Effl. R19 24	25
Components									
MeOH	0.88	0	0	0	0	0	0	0	0
PO	0	0	0.49	0.49	0.49	800.49	0.49	0.49	0.49
H2O	2.36	0	0	0	0	0	0	0	0
MP-1	5.13	1063.17	4521.56	5584.73	5584.73	5584.73	5584.73	4521.15	4521.15
MP-2	**10113.57**	**100.7**	**638.22**	**738.92**	**738.92**	**738.92**	**738.92**	**638.46**	**638.45**
MDP	**0**	**129.65**	**36.9**	**166.55**	**166.55**	**166.55**	**166.55**	**1960.94**	**1960.94**
MTP	0	0.61	0	0.61	0.61	0.61	0.61	167.44	167.44
PG	0	4.14	0.12	4.26	4.26	4.26	4.26	0.54	0.54
NaOCH3	0	38	0	38	38	38	38	38	38
DPG	0	0.62	0	0.62	0.62	0.62	0.62	7.18	7.18
M4P	0	0	0	0	0	0	0	0	0
Mass flow (kg/h)	10121.94	1336.89	5197.29	6534.18	6534.18	7334.18	6534.18	7334.20	7334.19
Enthalpy (MJ/h)	-47647.72	-5527.83	-22013.08	-27540.90	-28369.82	-28173.24	-26499.82	-30044.70	-30044.71

Appendix B2: List of stream compositions

Stream Number	26	Btms T21 27	28	29	30	31	32	33
Components								
MeOH	0	0	0.88	0	0	0.88	0	0
PO	0.49	0	0	0	0	0	0	0
H2O	0	0	2.36	0	0	2.36	0	0
MP-1	4521.56	0.99	5.13	0	0.99	5.13	0.99	0
MP-2	**638.22**	**0**	**10113.57**	**0**	**0**	**10113.57**	**0**	**0**
MDP	**36.9**	**1924.34**	**0**	**153.78**	**1770.57**	**0**	**1770.57**	**153.78**
MTP	0	167.44	0	157.87	12.57	0	12.57	154.87
PG	0.12	0.42	0	0	0.42	0	0.42	0
NaOCH3	0	38	0	38	0	~~38~~	0	38
DPG	0	7.21	0	5.48	1.73	0	1.73	5.48
M4P	0	0	0	0	0	0	0	0
Mass flow (kg/h)	5197.29	2138.40	10121.94	352.13	1786.28	10121.94	1786.28	352.13
Enthalpy (MJ/h)	-22023.50	-8555.82	-49445.28	-1345.87	-7201.64	-49444.14	-7823.00	-1487.59

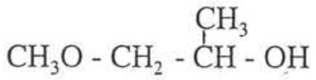
Appendix B2: List of stream compositions

Stream Number	34 MDP prod	35 Waste (HB[illegible]
Components		
MeOH	0	0
PO	0	0
H2O	0	0
MP-1	0.99	0
MP-2	**0**	**0**
MDP	**1770.57**	**153.78**
MTP	12.57	154.87
PG	0.42	0
NaOCH3	0	38
DPG	1.73	5.48
M4P	0	0
Mass flow (kg/h)	1786.28	352.13
Enthalpy (MJ/h)	-7822.80	-1487.56

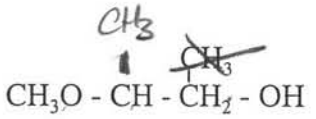
Appendix C1: Substances in the process

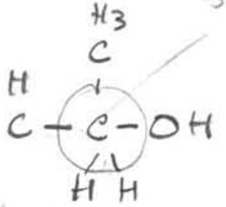
IUPAC Name	Molecular formula	Abbreviation	
Methanol	CH_3OH	MeOH	
1,2-Propylene oxide	$CH_3CH(O)CH_2$	PO	
1-Methoxy-2-propanol	$CH_3OCH_2CH(CH_3)OH$	MP-2	*
2-Methoxy-1-propanol	$CH_3OCH(CH_3)CH_2OH$	MP-1	
Methoxy-propoxy-propanol	$C_7H_{16}O_3$ (4 isomers)	MDP X	*
Methoxy-dipropoxy-propanol	$C_{10}H_{22}O_4$ (8 isomers)	MTP X	
Methoxy-tripropoxy-propanol	$C_{13}H_{28}O_5$ (16 isomers)	M4P X	
1,2-Propanediol	$HOCH_2CH(OH)CH_3$	PG V	
Dipropyleneglycol	$C_6H_{14}O_3$ (4 isomers)	DPG V	

1-Methoxy-2-propanol (MP-2):


$CH_3O - CH_2 - \overset{CH_3}{CH} - OH$

2-Methoxy-1-propanol (MP-1):

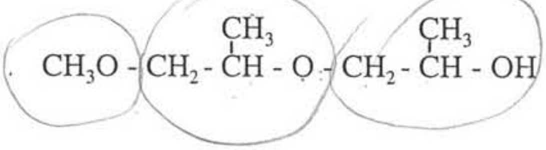

$CH_3O - \overset{CH_3}{CH} - \overset{\cancel{CH_3}}{CH_2} - OH$

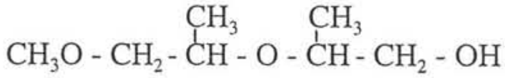


5 waardig?

Me x Prop x Prop ol

Methoxy-propoxy-propanol:
(two of four isomers)
(MDP)


$CH_3O - CH_2 - \overset{CH_3}{CH} - O - CH_2 - \overset{CH_3}{CH} - OH$


$CH_3O - CH_2 - \overset{CH_3}{CH} - O - \overset{CH_3}{CH} - CH_2 - OH$

MP2 + PO

iden

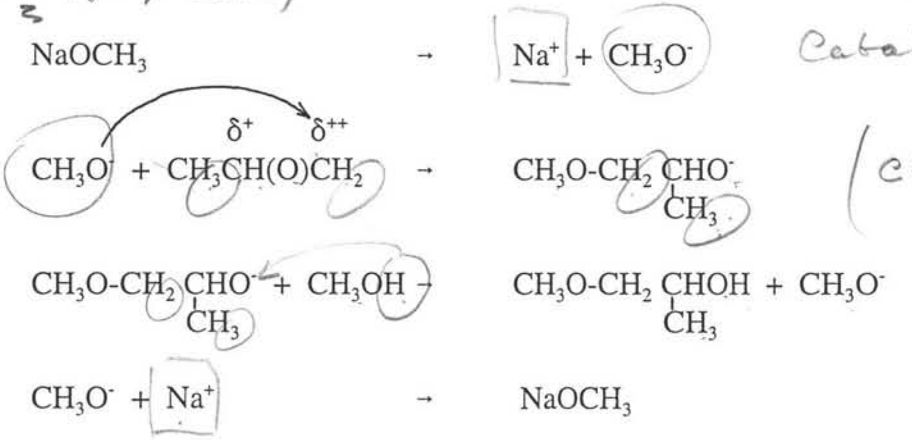
MP1 + PO

Appendix C2: Reaction mechanism

The following reactions were taken into account:

MeOH	+ PO	→	MP-2	[1]
MeOH	+ PO	→	MP-1	[2]
MP-2	+ PO	→	MDP	[3]
MP-1	+ PO	→	MDP	[4]
MDP	+ PO	→	MTP	[5]
H_2O	+ PO	→	PG	[6] x
PG	+ PO	→	DPG	[7] x
MTP	+ PO	→	M4P	[8]

The reaction mechanism is as follows and is applicable to all reaction numbers, except numbers 6 and 7. (glycols !)



$$NaOCH_3 \rightarrow Na^+ + CH_3O^-$$

Catalyst

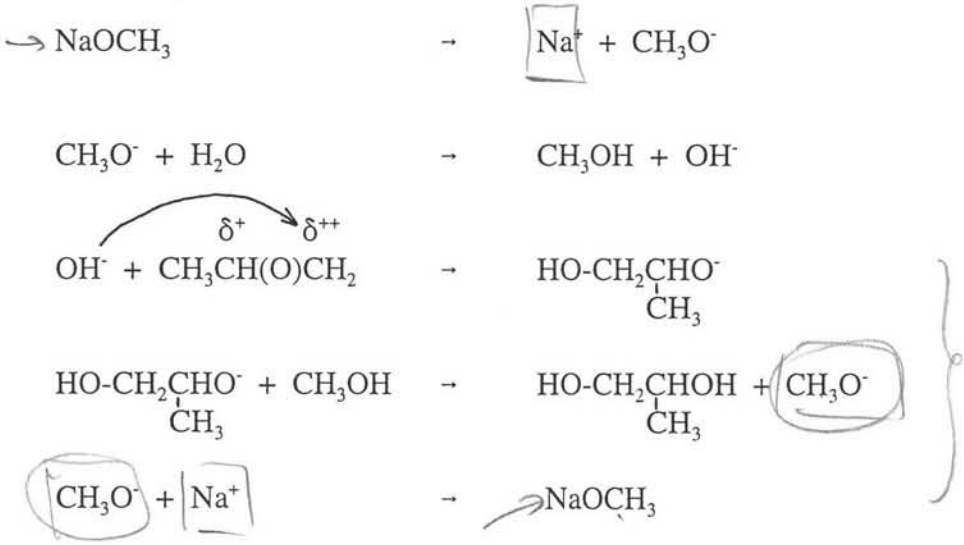
$$CH_3O^- + \overset{\delta^+}{CH_3CH}(O)\overset{\delta^{++}}{CH_2} \rightarrow CH_3O\text{-}CH_2\underset{CH_3}{CHO^-}$$

(CH₂ (O) CH CH₃)

$$CH_3O\text{-}CH_2\underset{CH_3}{CHO^-} + CH_3OH \rightarrow CH_3O\text{-}CH_2\underset{CH_3}{CHOH} + CH_3O^-$$

$$CH_3O^- + Na^+ \rightarrow NaOCH_3$$

For reaction number 6 and 7 the following mechanism is applicable:



$$NaOCH_3 \rightarrow Na^+ + CH_3O^-$$

$$CH_3O^- + H_2O \rightarrow CH_3OH + OH^-$$

$$OH^- + \overset{\delta^+}{CH_3CH}(O)\overset{\delta^{++}}{CH_2} \rightarrow HO\text{-}CH_2\underset{CH_3}{CHO^-}$$

$$HO\text{-}CH_2\underset{CH_3}{CHO^-} + CH_3OH \rightarrow HO\text{-}CH_2\underset{CH_3}{CHOH} + CH_3O^-$$

$$CH_3O^- + Na^+ \rightarrow NaOCH_3$$

Note: When using NaOH as catalyst the last three reactions are applicable, resulting in formation of unwanted propylene glycols.

Appendix D: Reactions with kinetic data

The following reactions were taken into account. The reference temperature for heat of reaction is 430 K. These values were calculated with standard heat of formation and heat capacity-temperature relations.

MeOH + PO → MP-2 ΔH_r = -103 kJ/mol [1] = [6]
MeOH + PO → MP-1 ΔH_r = - 95 kJ/mol [2]
MP-2 + PO → MDP ΔH_r = -106 kJ/mol [3] = [7]
MP-1 + PO → MDP ΔH_r = -114 kJ/mol [4]
MDP + PO → MTP ΔH_r = -113 kJ/mol [5]
H_2O + PO → PG ΔH_r = - 78 kJ/mol [6] ς = [1]
PG + PO → DPG ΔH_r = -119 kJ/mol [7] ς = [3]
MTP + PO → M4P ΔH_r = -113 kJ/mol [8]

In the following table kinetic data of the reactions mentioned above is given. With the Arrhenius relation and this kinetic data, reaction rate constants can be calculated.

Ko EA

Reaction number	Pre-exponential constant ($l^2/mol^2.s$)	Activation energy (kJ/mol)
1 ✓	1.50E+08 1 50,000,0E + 3	74.0
2	1.80E+09 1 800,000,0 E + 3	85.0
3	6.70E+06 6,700,0 E + 3	70.0
4	5.80E+04 58,0 E + 3	69.0
5	4.70E+04 47,0 E + 3	63.0
6 ✓	1.50E+08 150,000.0 E + 3	74.0
7	6.70E+06 6,700.0 E + 3	70.0
8	6.50E+03 6.5 E+3	62.0

EA

Table D.1: Kinetic data

Appendix E1.1

Mass and energy balances reactors

MP-2 reactor (Equipment nr 5)

DIFFERENTIAL EQUATIONS:

$$d(T)/d(TAU) = (-UA(T-Tfeed)/vb+(k1\cdot ca\cdot cb\cdot ckat+k2\cdot ca\cdot cb\cdot ckat+k3\cdot ca\cdot cc\cdot ckat+k4\cdot ca\cdot cd\cdot ckat+ k5\cdot ca\cdot ce\cdot ckat+k1\cdot ca\cdot cf\cdot ckat+k1\cdot ca\cdot cg\cdot ckat+k5\cdot ca\cdot ch\cdot ckat)\cdot -1\cdot DHr)/((ca\cdot cpa+ cb\cdot cpb+cc\cdot cpc+cd\cdot cpc+ce\cdot cpe+cf\cdot cpf+cg\cdot cpg+ch\cdot cph)) \qquad (4.4)$$

$$d(TFEED)/d(TAU) = (UA\cdot(T-Tfeed)/vb)/((ca0\cdot cpa+cb0\cdot cpb+cc0\cdot cpc+cd0\cdot cpC+ce0\cdot cpe+ cf0\cdot cpf+cg0\cdot cpg+ch0\cdot cph0)) \qquad (4.5)$$

$$d(CA)/d(TAU)= -(k1\cdot ca\cdot cb\cdot ckat+k2\cdot ca\cdot cb\cdot ckat+k3\cdot ca\cdot cc\cdot ckat+k4\cdot ca\cdot cd\cdot ckat+ k5\cdot ca\cdot ce\cdot ckat+k1\cdot ca\cdot cf\cdot ckat+k1\cdot ca\cdot cg\cdot ckat+k5\cdot ca\cdot ch\cdot ckat)$$

$$d(CB)/d(TAU) = -(k1\cdot ca\cdot cb\cdot ckat+k2\cdot ca\cdot cb\cdot ckat)$$

$$d(CC)/d(TAU) = (k1\cdot ca\cdot cb\cdot ckat-k3\cdot ca\cdot cc\cdot ckat)$$

$$d(CD)/d(TAU) = (k2\cdot ca\cdot cb\cdot ckat-k4\cdot ca\cdot cd\cdot ckat)$$

$$d(CE)/d(TAU) = (k3\cdot ca\cdot cc\cdot ckat+k4\cdot ca\cdot cd\cdot ckat-k5\cdot ca\cdot ce\cdot ckat)$$

$$d(CF)/d(TAU) = -(k1\cdot cf\cdot ca\cdot ckat)$$

$$d(CG)/d(TAU) = (k1\cdot cf\cdot ca\cdot ckat-k1\cdot ca\cdot cg\cdot ckat)$$

$$d(CH)/d(TAU) = (k5\cdot ca\cdot ce\cdot ckat-k5\cdot ca\cdot ch\cdot ckat)$$

$K1 = K_{0,1}\cdot \exp(-E_{A1}/(T\cdot 8.314))$
$K2 = K_{0,2}\cdot \exp(-E_{A2}/(T\cdot 8.314))$
$K3 = K_{0,3}\cdot \exp(-E_{A3}/(T\cdot 8.314))$
$K4 = K_{0,4}\cdot \exp(-E_{A4}/(T\cdot 8.314))$
$K5 = K_{0,5}\cdot \exp(-E_{A5}/(T\cdot 8.314))$
$CPA = (1.651e5-6.295e2\cdot T+2.011\cdot T\text{^}2-1.308E-3\cdot T\text{^}3)/1000$
$CPB = (1.058E5-3.622E2\cdot T+9.379E-1\cdot T\text{^}2)/1000$
$CPC = (1.541E5+2.134E2\cdot T)/1000$
$CPE = (2.066E5+4.202E2\cdot T)/1000$
$CPF = (2.764E5-2.090E3\cdot T+8.125\cdot T\text{^}2-1.412E-2\cdot T\text{^}3+9.370E-6\cdot T\text{^}4)/1000$
$CPG = (5.808E4+4.452E2\cdot T)/1000$
$CPH = (2.602E5+6.082E2\cdot T)/1000$

Where A or a=PO
B or b=MeOH
C or c=MP-2
D or d=MP-1
E or e=MDP
F or f=H_2O
G or g=PG
H or h=MTP
kat=catalyst
'0'=in the feed

TAU=residence time (s)
vb=reactor volume (l)
c=concentration (mol/l)
Dhr=overall heat of reaction (J/mol)
CP=specific heat (J/molK)

Appendix E1.1

Mass and energy balances reactors

MDP reactor (Equipment nr 19)

DIFFERENTIAL EQUATION(S):

d(T)/d(TAU) =(-UA·(T-Tfeed)/Vbuis+(k3·ca·cc·ckat+k4·ca·cd·ckat+k5·ca·ce·ckat+k7·ca·cg·ckat+k5·ca·ch·ckat)·-1·DHr)/(ca·cpa+cc·cpc+cd·cpC+ce·cpe+cg·cpg+ch·cph+ci·cpi+cj·cpj+CKAT·cpkat)

d(TFEED)/d(TAU) = (UA·(T-Tfeed)/Vbuis)/(ca0·cpa+cc0·cpc+cd0·cpC+ce0·cpe+cg0·cpg+ch0·cph+ci0·cpi+cj0·cpj+ckat·cpkat)

d(CA)/d(TAU) = -(k3·ca·cc·ckat+k4·ca·cd·ckat+k5·ca·ce·ckat+k7·ca·cg·ckat+k5·ca·ch·ckat)

d(CC)/d(TAU) = -(k3·ca·cc·ckat)

d(CD)/d(TAU) = -(k4·ca·cd·ckat)

d(CE)/d(TAU) = (k3·ca·cc·ckat+k4·ca·cd·ckat-k5·ca·ce·ckat)

d(CG)/d(TAU) = -(k7·ca·cg·ckat)

d(CH)/d(TAU) = (k5·ca·ce·ckat-k5·ca·ch·ckat)

d(CI)/d(TAU) = (k5·ch·ca·ckat)

d(CJ)/d(TAU) = (k7·ca·cg·ckat)

K3 = $K_{0,3}$·exp(-$E_{A,3}$/(T·8.314))
K4 = $K_{0,4}$·exp(-$E_{A,4}$/(T·8.314))
K5 = $K_{0,5}$·exp(-$E_{A,5}$/(T·8.314))
K7 = $K_{0,7}$·exp(-$E_{A,7}$/(T·8.314))
CPA = (1.651e5-6.295E2·T+2.011·T^2-1.308E-3·t^3)/1000
CPC = (1.541E5+2.134E2·T)/1000
CPE = (2.066E5+4.202E2·T)/1000
CPG = (5.808E4+4.452E2·T)/1000
CPH = (2.602E5+6.082E2·T)/1000
CPI = (2.602E5+6.082E2·T)/1000
CPJ = (1.414E5+6.195E2·T)/1000
CPKAT = (8.756E4+3.970E-1·T-6.380E-3·T^2+2.439E-6·T^3+2.571E-10·T^4)/1000

Where A or a=PO
C or c=MP-2
D or d=MP-1
E or e=MDP
G or g=PG
H or h=MTP
I or i=M4P
J or j=DPG
'0'=in the feed

TAU=residence time (s)
c=concentration (mol/l)
Dhr=overall heat of reaction (J/mol)
vb=reactor volume (l)
CP=specific heat (J/molK)

Appendix E 1.2

Calculation of the stochiometric coefficients and the overall heat of reaction

Reactor 1 *MeOH + PO + H2O -> MP2 + MP1 + MDP + MTP + M4P + PG + DPG*

	molar flow IN kmol/h	molar flow OUT kmol/h		stoichiometric coefficient nu
MeOH	7.77E+02	6.51E+02	MeOH	-9.92E-01
PO	1.27E+02	1.16E-01	PO	-1.00E+00
H2O	4.70E-01	4.00E-01	H2O	-5.47E-04
MP2	2.44E-05	1.13E+02	MP2	8.92E-01
MDP	0.00E+00	8.77E-01	MDP	6.91E-03
MTP	0.00E+00	2.99E-03	MTP	2.35E-05
PG	0.00E+00	6.41E-02	PG	5.05E-04
MP1	0.00E+00	1.19E+01	MP1	9.33E-02
DPG	0.00E+00	5.42E-03	DPG	4.27E-05
M4P	0.00E+00	7.57E-06	M4P	5.96E-08

	ΔH_f (kJ/mol)	nu*ΔH_f (kJ/mol)	**ΔH_R (kJ/mol)**
MeOH	-222.38	220.71	**-98.63**
PO	-99.42	99.42	
H2O	-275.55	0.15	
MP2	-421.14	-375.75	
MDP	-625.29	-4.32	
MTP	-835.92	-0.02	
DIOL	-452.80	-0.23	
MP1	-413.30	-38.57	
DPG	-671.48	-0.03	
M4P	-1046.57	0.00	

Reactor 2 *PO+ MP2 + MP1+ PG -> MDP + MTP + M4P + DPG*

	molar flow IN (kmol/h)	molar flow OUT (kmol/h)		stoichiometric coefficient nu
MeOH	0.00E+00	0.00E+00	MeOH	0.00E+00
PO	1.38E+01	8.13E-03	PO	-1.00E+00
H2O	0.00E+00	0.00E+00	H2O	0.00E+00
MP2	8.19E+00	7.08E+00	MP2	-8.08E-02
MDP	1.13E+00	1.32E+01	MDP	8.78E-01
MTP	2.99E-03	8.11E-01	MTP	5.86E-02
PG	6.79E-02	8.65E-03	PG	-4.30E-03
MP1	6.20E+01	5.02E+01	MP1	-8.56E-01
DPG	5.54E-03	6.47E-02	DPG	4.30E-03
M4P	7.57E-06	7.57E-06	M4P	0.00E+00

	ΔH_f (kJ/mol)	nu*ΔH_f (kJ/mol)	**ΔH_R (kJ/mol)**
MeOH	-218.51	0.00	**-112.58**
PO	-95.02	95.02	
H2O	-273.83	0.00	
MP2	-412.62	33.33	
MDP	-613.80	-539.19	
MTP	-820.68	-48.12	
PG	-446.46	1.92	
MP1	-405.59	347.30	
DPG	-661.44	-2.84	
M4P	-1027.59	0.00	

Appendix E 1.3 Reactor design

	MP-2 reactor	***MDP-reactor***		
equipment number	***R5***	***R19***		
type	shell and tube floating head	shell and tube floating head		
tube-side medium	reaction mixture	reaction mixture		
shell-side medium	feed	feed		
number of tube-side passes	6	6	-	
number of shell-side passes	1	1	-	
Results from Chemcad:				
Phi$_m$ tube	32332.5	7336.4	kg/h	
Phim shell	32332.5	7336.4	kg/h	
C_p tube	3.51	2.76	kJ/kgC	
C_p shell	3.11	2.66	kJ/kgC	
k tube	0.15	0.11	W/mC	
k shell	0.17	0.12	W/mC	
Rho tube	647.42	771.25	kg/m^3	
Rho shell	696.31	800.49	kg/m^3	
Viscosity tube	0.22	0.18	mPas	
Viscosity shell	0.26	0.21	mPas	
Results from mass and energy balance:				
V	7.0	1.2	m^3	
T tube-side in	126.9	167.9	C	
T tube-side out	152.1	99.9	C	
T shell-side in	53.7	174.3	C	
T shell-side out	139.7	167.4	C	
U*A	60000	10000	W/C	
delta T_m	45.2	38.8	C	
Q	2.712	0.388	MW	
U estimated	82.0	82.0	W/m^2C	
A	731.71	121.95	m^2	
Values for tube diameter and tube length:				
d_o	0.050	0.050	m	
tube wall thickness	3.2	2.6	mm	
d_i	0.044	0.045	m	
L	10	10	m	
A, single tube	1.57	1.57	m^2	
Nt	466	78	-	
K_1	0.040	0.040		table 12.4 CR
n_1	2.617	2.617		table 12.4 CR
D_b	1.79	0.90	m	$D_b=d_o(N_t/K_1)^{1/n1}$
shell-bundle clearance	0.15	0.10	m	fig. 12.10 CR
shell diameter, D_s	1.94	1.00	m	D_b+shell bundle clearance

Appendix E 1.3 Reactor design

	MP-2 reactor	***MDP-reactor***		
equipment number	***R5***	***R19***		
Calculation of the tube-side heat transfer coefficient:				
Acr, single tube	1.49E-03	1.58E-03	m^2	
number of tubes per pass	78	13	-	
Acr,t	1.16E-01	2.04E-02	m^2	
G_t	77.48	99.91	kg/sm^2	$Phi_m / A_{cr,t}$
v	0.12	0.13	m/s	
Re	15568	24594	-	
Pr	5.11	4.69	-	
j_H	4.00E-03	3.90E-03	-	fig. 12.23 CR
h_i	364.61	381.43	W/m^{2}C	
Calculation of the shell-side heat transfer coefficient:				
l_B	1.02	0.35	m	
p_t	0.075	0.075	m	$1.5 * d_o$
Acr,s	0.658	0.115	m^2	$(p_t - d_o)/p_t * D_s * l_B$
G_s	13.66	17.71	kg/sm^2	$Phi_m / A_{cr,s}$
v	0.020	0.022	m/s	
d_e	0.093	0.093	m	
Re	4849	7698	-	
Pr	4.88	4.90	-	
baffle cut	25	25	%	
j_H	8.00E-03	7.00E-03	-	fig. 12.29 CR
h_o	117.48	113.54	W/m^{2}C	
Fouling coefficients:				
dirt coefficient tubes	5000	5000	W/m^{2}C	table 12.2 CR
dirt coefficient shell	5000	5000	W/m^{2}C	table 12.2 CR
1/U	1.22E-02	1.22E-02	m^{2}K/W	
U	82.22	81.85	W/m^{2}K	
Pressure drop:				
tube-side friction factor, jf	4.50E-03	3.80E-03		fig. 12.24 CR
ΔP_t	299	361	Pa	
shell-side friction factor, jf	5.50E-02	5.00E-02		fig. 12.30 CR
ΔP_s	12	24	Pa	

Appendix E 2.1: Overview Column Calculations

Performed for the top plate of the rectifying section, column T1.

Flow-rates and physical properties from ChemCad.

$\phi ml := 4910$ -liquid mass flow rate (kg/hr)

$\phi mv := 25780$ -vapour mass flow rate (kg/hr)

$\rho l := 748$ -liquid density (kg/m^3)

$\rho v := 1.18$ -vapour density (kg/m^3)

$\sigma := 0.019$ -surface tension (N/m)

Diameter calculations

Liquid-vapour flow factor:

$$Flv := \frac{\phi ml}{\phi mv} \cdot \sqrt{\frac{\rho v}{\rho l}} \qquad Flv = 0.008 \qquad \text{(eq. 4.17)}$$

tray spacing (m), C&R

$ts := 0.45$

from Fig. 11.27, C&R

$K1 := 0.073$

correction for surface tensions:

$$K := \left(\frac{\sigma}{0.02}\right)^{0.2} \cdot K1 \qquad K = 0.072$$

flooding vapour velocity (m/s), based on the net column cross-sectional area

$$uf := K \cdot \sqrt{\frac{\rho l - \rho v}{\rho v}} \qquad uf = 1.818 \qquad \text{(eq. 4.19)}$$

design for 85% flooding at maximum flow rate:

$$uv := uf \cdot 0.85 \qquad uv = 1.545$$

maximum volumetric flow rate (m^3/s):

$$\phi vmax := \frac{\phi mv}{\rho v \cdot 3600} \qquad \phi vmax = 6.069$$

net area required (m^2):

$$Anet := \frac{\phi vmax}{uv} \qquad Anet = 3.928$$

Column cross-sectioned area (downcomer area taken as 12% of total area (m^2)):

$$Acol := \frac{Anet}{1 - 0.12} \qquad Acol = 4.463$$

Column diameter (m)

$$dcol := \sqrt{\frac{4}{\pi} \cdot Acol} \qquad dcol = 2.384 \qquad \text{(eq. 4.18)}$$

Appendix E 2.1 (continued):

Provisional plate design:

Column diameter (m): $Dcol := 2.8$

Column area (m^2): $Acol := \frac{\pi}{4} \cdot Dcol^2$ $Acol = 6.158$

Downcomer area (m^2): $Ad := 0.12 \cdot Acol$ $Ad = 0.739$

Net area (m^2): $An := Acol - Ad$ $An = 5.419$

Active area (m^2): $Aa := Acol - 2 \cdot Ad$ $Aa = 4.68$

Hole area (m2):
(7.5% of active area) $Ah := 0.075 \cdot Aa$ $Ah = 0.351$

weir length lw (m) from figure 11.31, C&R:

$\frac{Ad}{Acol} \cdot 100 = 12$ $lw := 0.75 \cdot Dcol$ $lw = 2.1$

weir height (mm), C&R: $hw := 45$

hole diameter (mm), C&R: $Dh := 5$

plate thickness (mm),C&R: $tp := 5$

Perforated area:

wide unperforated edge strips round plate edge (m): $Wues := 50 \cdot 10^{-3}$

wide calming zones (m): $Wcz := 100 \cdot 10^{-3}$

from Fig. 11.32, C&R at

$\frac{lw}{Dcol} = 0.75$ $\theta c := 100$

angle subtended at plate edge by unperforated strips (°):

$\theta d := 180 - \theta c$ $\theta d = 80$

mean length, unperforated edge strips (m):

$mlues := (Dcol - Wues) \cdot \pi \cdot \frac{\theta d}{180}$ $mlues = 3.84$

area of unperforated edge strips (m^2):

$Aues := Wues \cdot mlues$ $Aues = 0.192$

area of calming zones (m^2):

$Acz := 2 \cdot Wcz \cdot (lw - 2 \cdot Wcz)$ $Acz = 0.38$

perforated area Ap (m^2):

$Ap := Aa - (Aues + Acz)$ $Ap = 4.108$

hole area/perforated area:

$\frac{Ah}{Ap} = 0.085$

hole pitch (lp/Dh)
from Fig. 11.33, C&R: $hp := 3.25$ satisfactory, within 2.5 to 4.

Appendix E 2.1 (continued):

Number of holes:

number of holes:

$N := \frac{Ah}{\frac{\pi}{4} \cdot \left(Dh \cdot 10^{-3}\right)^2}$ $\quad N = 1.788 \cdot 10^4$

hole diam?

Rectification section design:

-check weeping

maximum liquid rate (kg/s):

$max\phi ml := \frac{\phi ml}{3600}$ $\quad max\phi ml = 1.364$

minimum liquid rate (kg/s), at 70% turn down:

$min\phi ml := 0.70 \cdot max\phi ml$ $\quad min\phi ml = 0.955$

clear liquid depth (mm liquid):

$howmax := 750 \cdot \left(\frac{max\phi ml}{\rho l \cdot lw}\right)^{\frac{2}{3}}$ $\quad howmax = 6.826$ (eq. 4.20)

$howmin := 750 \cdot \left(\frac{min\phi ml}{\rho l \cdot lw}\right)^{\frac{2}{3}}$ $\quad howmin = 5.381$ (eq. 4.20)

form Fig. 11.30, C&R:

$hw + howmin = 50.381$ $\quad K2 := 30.0$

minimum vapour velocity (m/s):

$uhmin := \frac{(K2 - 0.90 \cdot (25.4 - Dh))}{\sqrt{(\rho v)}}$ $\quad uhmin = 10.715$ (eq. 4.19)

actual minimum vapour velocity (m/s):

$uhminactual := 0.70 \cdot \frac{\phi vmax}{Ah}$ $\quad uhminactual = 12.104$

The actual minimum vapour velocity (uhminactual) exceeds the minimum vapour velocity (uhmin). Therefore the minimum operating rate will be well above weep point.

Plate pressure drop

Dry plate drop
Maximum vapour velocity through holes (m/s):

$uh := \frac{\phi vmax}{Ah}$ $\quad uh = 17.291$

Orifice coefficient (Co)

hole pitch (m), C&R:

$lp := 3.25 \cdot Dh$ $\quad lp = 16.25$

Appendix E 2.1 (continued):

From Fig. 11.34:

for plate thickness/hole diameter = $\frac{tp}{Dh} = 1$ and $\frac{Ah}{Ap} \cdot 100 = 8.544$ $Co := 0.84$

Dry plate drop (mm liquid):

$hd := 51 \cdot \left(\frac{uh}{Co}\right)^2 \cdot \frac{\rho v}{\rho l}$ $hd = 34.09$ (eq. 4.22)

residual head (mm liquid):

$hr := \frac{12500}{\rho l}$ $hr = 16.711$ (eq. 4.23)

Total plate drop (mm liquid):

$ht := hd + (hw + howmin) + hr$ $ht = 101.183$ (eq. 4.21)

Downcomer design (back-up):

Downcomer pressure loss:

height of the bottom edge of the apron above the plate (mm):

$hap := hw - 10$ $hap = 35$

clearance area under the downcomer (m^2):

$Aap := \frac{hap}{1000} \cdot lw$ $Aap = 0.073$

$Ad = 0.739$

As Aap is less than Ad, therefore Aap is used in the next equation:

head loss in the downcomer:

$hdc := 166 \cdot \left(\frac{\frac{\phi ml}{3600}}{\rho l \cdot Aap}\right)^2$ $hdc = 0.102$ (eq.4.25)

downcomer back-up in terms of clear liquid:

$hb := (hw + howmin) + ht + hdc$ $hb = 151.666$ (eq. 4.24)

froth height:

For safe design the clear liquid back-up (hb) should not exceed half the plate spacing (+ weir height), to avoid spacing:

$0.5 \cdot (ts \cdot 1000 + hw) = 247.5$ (eq. 4.26)

This is indeed the case, so tray spacing is acceptable

check residence time (sec):

$tr := \frac{Ad \cdot hb \cdot \rho l}{\phi ml}$ $tr = 17.072$ (eq. 4.27)

The residence time in the downcomer must be at least 3 seconds to allow the entrained vapour to disengage from the liquid stream.

Appendix E 2.1 (continued):

Check entrainment

actual velocity (based on net area):

$uv := \frac{\phi vmax}{An}$ $\quad$ $uv = 1.12$

per cent flooding

$\frac{uv}{uf} \cdot 100 = 61.613$

As the per cent flooding is well bellow the design figure of 85, the column diameter could be reduced, but this would increase the pressure drop.

from figure 11.29, C&R:

$Flv = 0.008$ gives entrainment $\psi := 0.11$

entrainment should be less than 0.1 in order to neglect entrainment effects on the plate efficiency.

Appendix E 2.2a: Results Calculations Column T7

CHEMCAD data

	rectifying section		stripping section	
	top	bottom	top	bottom
tray	2	19	20	26
ϕml (kg/h)	4910	6668	33459	63710
ϕmv (kg/h)	25782	27280	27532	51217
ϕml (kg/s)	1.36	1.85	9.29	17.70
ϕmv (kg/s)	7.16	7.58	7.65	14.23
ρl (kg/m^3)	748.6	791.94	795.97	784.83
ρv (kg/m^3)	1.2	1.5	1.5	3.6
σ (N/m)	0.019	0.019	0.019	0.014

Column height

Ecol (%)	80			
	N theor.	N real	tray spacing (m)	height (m)
rectifying	18	23	0.45	10.35
stripping	7	9	0.45	4.05
total	25	32		14.40

column height (m) = 1.15 * total height : 16.56

calculation column diameter

Flv (-)	0.008	0.011	0.053	0.085
tray spacing (m)	0.45	0.45	0.45	0.45
K1	0.073	0.078	0.080	0.077
K	0.072	0.077	0.079	0.072
uf (m/s)	1.818	1.790	1.828	1.050
uv (m/s)	1.546	1.522	1.554	0.893
Qvmax (m^3/s)	6.069	5.155	5.133	3.909
Anet (m^2)	3.926	3.388	3.303	4.378
Acol (m^2)	4.462	3.849	3.753	4.975
Dcol (m)	2.384	2.214	2.186	2.517

Provisional plate design

Dcol (m)	2.800	2.800	2.800	2.800
Acol (m^2)	6.158	6.158	6.158	6.158
Ad (m^2)	0.739	0.739	0.739	0.739
An (m^2)	5.419	5.419	5.419	5.419
Aa (m^2)	4.680	4.680	4.680	4.680
Ah (m^2)	0.351	0.351	0.351	0.351
Ad/Acol*100	12.0	12.0	12.0	12.0
lw/Dcol	0.75	0.75	0.75	0.75
lw (m)	2.100	2.100	2.100	2.100
hw (mm)	45	45	45	45
Dh (mm)	5	5	5	5
tp (mm)	5	5	5	5

Perforated area

Wues (m)	5.00E-02	5.00E-02	5.00E-02	5.00E-02
Wcz (m)	1.00E-01	1.00E-01	1.00E-01	1.00E-01
θc (°)	100	100	100	100
θd (°)	80	80	80	80
mlues (m)	3.840	3.840	3.840	3.840
Aues (m^2)	0.192	0.192	0.192	0.192
Acz (m^2)	0.380	0.380	0.380	0.380
Ap (m^2)	4.108	4.108	4.108	4.108
lp/Dh	3.25	3.25	3.25	3.25
lp (mm)	16.2	16.2	16.2	16.2

Number of holes

N	17875	17875	17875	17875

check weeping

ϕml,min (kg/s)	0.955	1.297	6.506	12.388
how,min (mm)	5.379	6.353	18.558	28.778
hw+how,min (mm)	50.379	51.353	63.558	73.778
K2	30	30.1	30.4	30.7
uh,min (m/s)	10.715	9.683	9.864	6.468
uh,min actual (m/s)	12.105	10.281	10.237	7.795

plate pressure drop

uh,max (m/s)	17.3	14.7	14.6	11.1
tp/Dh	1.0	1.0	1.0	1.0
Ah/Ap*100	8.5	8.5	8.5	8.5
Co (-)	0.84	0.84	0.84	0.84
hd (mm)	34.5	29.3	29.3	42.1
hr (mm)	16.7	15.8	15.7	15.9
ht (mm)	101.6	96.4	108.5	131.8

downcomer design

hap (mm)	35	35	35	35
Aap (m^2)	0.074	0.074	0.074	0.074
Ad (m^2)	0.739	0.739	0.739	0.739
hdc (mm)	0.1	0.2	4.2	15.6
hbc (mm)	152.0	147.9	176.3	221.2
froth height (mm)	247.5	247.5	247.5	247.5

check residence time

tr (sec)	11.7	11.4	13.6	9.0

check entrainment

uv (m/s)	1.120	0.951	0.947	0.721
% flooding	61.6	53.1	51.8	68.7
Flv	0.008	0.011	0.053	0.085
entrainment	0.11	0.07	0.019	0.035

Appendix E 2.2b: Results Calculations Column T12

CHEMCAD data

	rectifying section		stripping section			
	top	bottom	top			bottom
tray	2	37	38	56	57	65
ϕml (kg/h)	49875	53451	65793	101965	113677	438424
ϕmv (kg/h)	60023	63267	63823	91845	100628	412539
ϕml (kg/s)	13.9	14.8	18.3	28.3	31.6	121.8
ϕmv (kg/s)	16.7	17.6	17.7	25.5	28.0	114.6
ρl (kg/m^3)	778.8	771.2	771.52	801.3	803.6	824.6
ρv (kg/m^3)	3.7	4.6	4.6	5.0	5.0	5.2
σ (N/m)	0.014	0.013	0.013	0.014	0.014	0.016

Column height

Ecol (%)	80			
	N theor.	N real	tray spacing (m)	height (m)
rectifying	36	45	0.5	22.5
stripping	19	24	0.5	12.00
	9	11	0.7	7.70
total	64	80		42.2

column height (m) = 1.15 * total height : 48.53

calculation column diameter

Flv (-)	5.7E-02	6.5E-02	8.0E-02	8.7E-02	8.9E-02	8.5E-02
tray spacing (m)	0.5	0.5	0.5	0.5	0.7	0.7
K1	8.9E-02	8.8E-02	8.5E-02	8.3E-02	8.2E-02	8.5E-02
K	8.3E-02	8.1E-02	7.8E-02	7.7E-02	7.6E-02	8.1E-02
uf (m/s)	1.21	1.04	1.01	0.97	0.97	1.01
uv (m/s)	1.02	0.89	0.85	0.83	0.82	0.86
Qvmax (m^3/s)	4.55	3.83	3.84	5.14	5.60	21.86
Anet (m^2)	4.44	4.32	4.49	6.22	6.82	25.45
Acol (m^2)	5.05	4.90	5.11	7.06	7.75	28.92
Dcol (m)	2.54	2.50	2.55	3.00	3.14	6.07

Provisional plant design

Dcol (m)	3.00	3.00	3.00	3.00	6.07	6.07
Acol (m^2)	7.07	7.07	7.07	7.06	28.94	28.94
Ad (m^2)	0.85	0.85	0.85	0.85	3.47	3.47
An (m^2)	6.22	6.22	6.22	6.22	25.47	25.47
Aa (m^2)	5.37	5.37	5.37	5.37	21.99	21.99
Ah (m^2)	0.46	0.46	0.46	0.54	0.70	2.75
Ad/Acol*100	12.00	12.00	12.00	12.00	12.00	12.00
lw/Dcol	0.75	0.75	0.75	0.75	0.75	0.75
lw (m)	2.25	2.25	2.25	2.25	4.55	4.55
hw (mm)	45.00	45.00	45.00	45.00	50.00	50.00
Dh (mm)	5.00	5.00	5.00	5.00	5.00	5.00
tp (mm)	5.00	5.00	5.00	5.00	5.00	5.00

Perforated area

Wues (m)	0.050	0.050	0.050	0.050	0.050	0.050
Wcz (m)	0.100	0.100	0.100	0.100	0.100	0.100
θc (°)	100.0	100.0	100.0	100.0	100.0	100.0
θd (°)	80.0	80.0	80.0	80.0	80.0	80.0
mlues (m)	4.1	4.1	4.1	4.1	8.4	8.4
Aues (m^2)	0.2	0.2	0.2	0.2	0.4	0.4
Acz (m^2)	0.4	0.4	0.4	0.4	0.9	0.9
Ap (m^2)	4.8	4.8	4.8	4.8	20.7	20.7
lp/Dh	3.1	3.1	3.1	2.8	5.1	2.6033
lp (mm)	15.3	15.3	15.3	14.1	25.7	13.0

Number of holes

N	23256	23256	23256	27339	35843	140011

check weeping

ϕml,min (kg/s)	9.7	10.4	12.8	19.8	22.1	85.2
how,min (mm)	23.5	24.7	28.4	37.1	24.9	60.1
hw+how,min (mm)	68.5	69.7	73.4	82.1	74.9	110.1
K2	30.5	30.5	30.8	30.8	30.8	31.1
uh,min (m/s)	6.3	5.7	5.8	5.6	5.5	5.6
uh,min actual (m/s)	7.0	5.9	5.9	6.7	5.6	5.6

plate pressure drop

uh,max (m/s)	10.0	8.4	8.4	9.6	8.0	8.0
tp/Dh	1.0	1.0	1.0	1.0	1.0	1.0
Ah/Ap*100	9.6	9.6	9.6	11.3	3.4	13.3
Co (-)	0.84	0.84	0.84	0.85	0.86	0.87
hd (mm)	33.8	30.2	30.6	40.1	27.4	27.1
hr (mm)	16.1	16.2	16.2	15.6	15.6	15.2
ht (mm)	118.3	116.2	120.2	137.8	117.9	152.4

downcomer design

hap (mm)	35.0	35.0	35.0	35.0	40.0	40.0
Aap (m^2)	0.1	0.1	0.1	0.1	0.2	0.2
Ad (m^2)	0.8	0.8	0.8	0.8	3.5	3.5
hdc (mm)	8.5	9.9	15.0	33.5	7.7	109.2
hbc (mm)	195.2	195.8	208.6	253.4	200.5	371.7
froth height (mm)	272.5	272.5	272.5	272.5	375.0	375.0

check residence time

tr (sec)	9.3	8.6	7.5	6.1	17.7	8.7

check entrainment

uv (m/s)	0.73	0.62	0.62	0.83	0.22	0.86
% flooding	61	59	61	85	23	85
Flv	0.057	0.065	0.080	0.087	0.089	0.085
entrainment	0.065	0.062	0.048	0.048	0.048	0.044

Appendix E 2.2c: Results Calculations Column T21

CHEMCAD data

	rectifying section		stripping section	
	top	bottom	top	bottom
tray	2	14	15	28
ϕml (kg/h)	11324	2316	4916	4202
ϕmv (kg/h)	17048	7578	7516	2078
ϕml (kg/s)	3.15	0.64	1.37	1.17
ϕmv (kg/s)	4.74	2.11	2.09	0.58
ρl (kg/m^3)	855.7	823.1	826.1	762.4
ρv (kg/m^3)	2.8	3.3	3.3	5.1
σ (N/m)	0.02	0.016	0.016	0.011

Column height

Ecol (%)	80			
	N theor.	N real	tray spacing (m)	height (m)
rectifying	13	17	0.55	9.35
stripping	14	18	0.55	9.90
total	27	35		19.25
	column height (m) = 1.15 * total height :			22.14

calculation column diameter

Flv (-)	0.038	0.019	0.041	0.165
tray spacing (m)	0.55	0.55	0.55	0.55
K1	0.100	0.100	0.100	0.081
K	0.100	0.096	0.096	0.072
uf (m/s)	1.744	1.518	1.516	0.876
uv (m/s)	1.482	1.290	1.289	0.745
Qvmax (m^3/s)	1.689	0.647	0.638	0.113
Anet (m^2)	1.139	0.501	0.495	0.152
Acol (m^2)	1.266	0.557	0.562	0.173
Dcol (m)	1.270	0.842	0.846	0.469

Provisional plate design

Dcol (m)	1.300	1.300	0.850	0.850
Acol (m^2)	1.327	1.327	0.567	0.567
Ad (m^2)	0.133	0.133	0.068	0.068
An (m^2)	1.195	1.195	0.499	0.499
Aa (m^2)	1.062	1.062	0.431	0.431
Ah (m^2)	0.159	0.064	0.052	0.013
Ad/Acol*100	10.0	10.0	12.0	12.0
lw/Dcol	0.72	0.72	0.75	0.75
lw (m)	0.936	0.936	0.638	0.638
hw (mm)	45	45	45	45
Dh (mm)	5	5	5	5
tp (mm)	5	5	5	5

Perforated area

Wues (m)	5.00E-02	5.00E-02	5.00E-02	5.00E-02
Wcz (m)	1.00E-01	1.00E-01	1.00E-01	1.00E-01
θc (°)	100	100	100	100
θd (°)	80	80	80	80
mlues (m)	1.745	1.745	1.117	1.117
Aues (m^2)	0.087	0.087	0.056	0.056
Acz (m^2)	0.147	0.147	0.088	0.088
Ap (m^2)	0.827	0.827	0.288	0.288
lp/Dh	2.16	3.42	2.24	4.48
lp (mm)	10.8	17.1	11.2	22.4

Number of holes

N	8112	3245	2636	659

check weeping

ϕml,min (kg/s)	2.202	0.450	0.956	0.817
how,min (mm)	14.718	5.243	11.160	10.604
hw+how,min (mm)	59.718	50.243	56.160	55.604
K2	30.35	30	30.3	30.3
uh,min (m/s)	7.160	6.451	6.600	5.291
uh,min actual (m/s)	7.422	7.104	8.628	6.132

plate pressure drop

uh,max (m/s)	10.603	10.149	12.326	8.760
tp/Dh	1.00	1.00	1.00	1.00
Ah/Ap*100	19.3	7.7	18.0	4.5
Co (-)	0.91	0.83	0.91	0.8
hd (mm)	22.7	30.2	37.1	40.9
hr (mm)	14.6	15.2	15.1	16.4
ht (mm)	97.0	95.6	108.4	112.8

downcomer design

hap (mm)	35	35	35	35
Aap (m^2)	0.033	0.033	0.022	0.022
Ad (m^2)	0.133	0.133	0.068	0.068
hdc (mm)	2.1	0.1	0.9	0.8
hbc (mm)	158.8	145.9	165.4	169.2
froth height (mm)	297.5	297.5	297.5	297.5

check residence time

tr (sec)	5.7	24.8	6.8	7.5

check entrainment

uv (m/s)	1.414	0.541	1.277	0.227
% flooding	81.06	35.66	84.24	25.90
Flv	0.038	0.019	0.041	0.165
entrainment	0.17	0.0075	0.19	0.002

Appendix E 2.2d: Results Calculations Column T28

CHEMCAD data

	rectifying section		stripping section	
	top	bottom	top	bottom
tray	2	5	6	10
ϕml (kg/h)	290	250	2409	2172
ϕmv (kg/h)	2087	2062	2036	2022
ϕml (kg/s)	0.08	0.07	0.67	0.60
ϕmv (kg/s)	0.58	0.57	0.57	0.56
ρl (kg/m^3)	759.2	758	762.3	761.5
ρv (kg/m^3)	5.2	5.3	5.3	5.5
σ (N/m)	0.011	0.011	0.01	0.01

Column height

Ecol (%)	80			
	N theor.	N real	tray spacing (m)	height (m)
rectifying	4	5	0.5	2.50
stripping	5	7	0.5	3.50
total	9	12		6.00
	column height (m) = 1.15 * total height :			6.90

calculation column diameter

Flv (-)	0.011	0.010	0.099	0.091
tray spacing (m)	0.50	0.50	0.50	0.50
K1	0.083	0.081	0.080	0.082
K	0.074	0.072	0.070	0.071
uf (m/s)	0.891	0.858	0.832	0.838
uv (m/s)	0.757	0.729	0.707	0.712
Qvmax (m^3/s)	0.113	0.108	0.107	0.102
Anet (m^2)	0.149	0.149	0.151	0.144
Acol (m^2)	0.169	0.169	0.171	0.163
Dcol (m)	0.464	0.464	0.467	0.456

Provisional plant design

Dcol (m)	0.540	0.540	0.540	0.540
Acol (m^2)	0.229	0.229	0.229	0.229
Ad (m^2)	0.027	0.027	0.027	0.027
An (m^2)	0.202	0.202	0.202	0.202
Aa (m^2)	0.174	0.174	0.174	0.174
Ah (m^2)	0.014	0.014	0.014	0.014
Ad/Acol*100	12.0	12.0	12.0	12.0
lw/Dcol	0.75	0.75	0.75	0.75
lw (m)	0.405	0.405	0.405	0.405
hw (mm)	45	45	45	45
Dh (mm)	5	5	5	5
tp (mm)	5	5	5	5

Perforated area

Wues (m)	5.00E-02	5.00E-02	5.00E-02	5.00E-02
Wcz (m)	7.50E-02	7.50E-02	7.50E-02	7.50E-02
θc (°)	100	100	100	100
θd (°)	80	80	80	80
mlues (m)	0.684	0.684	0.684	0.684
Aues (m^2)	0.034	0.034	0.034	0.034
Acz (m^2)	0.038	0.038	0.038	0.038
Ap (m^2)	0.102	0.102	0.102	0.102
lp/Dh	2.56	2.56	2.56	2.56
lp (mm)	12.8	12.8	12.8	12.8

Number of holes

N	709	709	709	709

check weeping

ϕml,min (kg/s)	0.056	0.049	0.468	0.422
how,min (mm)	2.421	2.195	9.903	9.249
hw+how,min (mm)	47.421	47.195	54.903	54.249
K2	29.9	29.9	30.2	30.2
uh,min (m/s)	5.085	5.022	5.138	5.053
uh,min actual (m/s)	5.659	5.453	5.354	5.143

plate pressure drop

uh,max (m/s)	8.084	7.791	7.649	7.347
tp/Dh	1.00	1.00	1.00	1.00
Ah/Ap*100	13.7	13.7	13.7	13.7
Co (-)	0.87	0.87	0.87	0.87
hd (mm)	29.9	28.5	27.5	26.2
hr (mm)	16.5	16.5	16.4	16.4
ht (mm)	93.8	92.2	98.8	96.9

downcomer design

hap (mm)	35	35	35	35
Aap (m^2)	0.014	0.014	0.014	0.014
Ad (m^2)	0.027	0.027	0.027	0.027
hdc (mm)	0.0	0.0	0.6	0.5
hbc (mm)	141.2	139.4	154.3	151.7
froth height (mm)	272.5	272.5	272.5	272.5

check residence time

tr (sec)	36.6	41.8	4.8	5.3

check entrainment

uv (m/s)	0.559	0.538	0.528	0.508
% flooding	63	63	64	61
Flv	0.011	0.010	0.099	0.091
entrainment	0.1	0.11	0.018	0.018

Appendix E 3. Heat exchanger calculations

Reboilers

Equipment number	H8 ✓	H13	H22	H29	
ype	thermosyphon horizontal	thermosyphon horizontal	thermosyphon horizontal	thermosyphon horizontal	
shell	cond. steam LP	cond. steam MP	cond. steam MP	steam MP	
ubes	MP2, MP1	MP1	MDP, MTP	MTP	
	fixed tube sheet	floating head	floating head	floating head	
eat duty (MW)	5.906	7.246	0.131	0.184	
T in shell	200	320	320 → 207	320	
T out shell	144	207	207	250	
T in tubes	130	155	201	230	
T out tubes	130	155	201	230	
Phi$_m$ shell (kg/s)	2.62	3.36	0.06	1.19	
Phi$_m$ tubes (kg/s)	14.55	121.41	0.41	0.51	
ΔTlm	34.79	97.86	38.00	46.54	
number of shell passes	1	1	1	1	
number of tube passes	2	2	2	2	
Ft	1	1	1	1	
ΔTm	34.79	97.86	38.00	46.54	
U (W/m2K)	1000	900	800	700	from table 12.1 C&R
A (m^2)	169.73	82.27	4.29	5.65	
di (m)	0.016	0.016	0.016	0.016	
do (m)	0.020	0.020	0.020	0.020	
L (m)	5	5	2.5	2.5	
tube wall material	AISI 304	AISI 304	AISI 304	AISI 304	
A heat transfer one tube (m^2)	0.31	0.31	0.16	0.16	
Nt	540	262	27	36	
Pt (square pitch) (m)	0.04	0.04	0.04	0.04	
K1	0.215	0.215	0.215	0.215	
n1	2.207	2.207	2.207	2.207	
Db (m)	0.69	0.50	0.18	0.20	
shell-bundle clearance (m)	0.015	0.058	0.053	0.054	
Ds (m)	0.71	0.56	0.23	0.26	
shell material	AISI 304	AISI 304	AISI 304	AISI 304	
pressure shell-side (bar)	4.0	18.0	18.0	18.0	
pressure tube-side (bar)	1.3	1.9	1.3	1.4	

Appendix E 3. Heat exchanger calculations

Condensers

Equipment number	H9	H15	H23	H30	
type	air condenser	air condenser	air condenser	air condenser	
tube-side medium	MeOH	MP2	MP1	MDP	
Heat duty (MW)	7.906	7.233	0.277	0.181	
T in tubes (C)	65	129	130	197	from ChemCad
T out tubes (C)	65	129	130	197	
Phi$_m$ tubes (kg/s)	7.18	16.70	4.74	0.58	
U (W/m2K)	425	425	425	425	
T air in (C)	23	23	23	23	from 'Brown'
T rise air (C)	16	40	40	65	
Correction factor temperature rise	0.8	0.8	0.8	0.8	
Corrected temperature rise (C)	12	32	32	52	from 'Brown'
T air out (C)	35	55	55	75	
LMTD (C)	34.9	89.0	89.9	146.6	
Correction factor LMTD	1	1	1	1	
Delta T	34.9	89.0	89.9	146.6	
A (m^2)	532.70	191.26	7.26	2.91	
di (m)	0.046	0.016	0.046	0.016	
do (m)	0.050	0.020	0.050	0.020	
L (m)	5	5	2	2.5	
tube wall material	carbon steel	carbon steel	carbon steel	carbon steel	
A bare tube	0.79	0.31	0.31	0.16	
number of bare tubes	678.26	608.80	23.12	18.50	
fan power (kW)	74.6	26.9	1.0	0.4	from 'Glass'
Pressure tubes (bar)	1.0	1.3	1.0	1.3	

Appendix E 3. Heat exchanger calculations

Coolers

Equipment number	H18	H26	H34	H33	
type	air cooler	air cooler	air cooler	air cooler	
tube-side medium	mainly MP1	MP2	MDP	mainly MTP	
heat duty (MW)	0.230	0.499	0.173	0.039	from ChemCad
T in tubes (C)	120	129	197	230	
T out tubes (C)	100	60	60	60	
Phi_m tubes (kg/s)	5.81	2.81	0.50	0.10	
U (W/m2K)	400.0	400.0	400.0	400.0	from 'Brown'
T air in (C)	23	23	23	23	
T rise air (C)	31	25	37	43	
correction factor temperature rise	0.90	0.96	1.02	1.04	from 'Brown'
corrected temperature rise (C)	27.58	24.13	37.96	44.67	
T air out (C)	50.6	47.1	61.0	67.7	
LMTD (C)	73.1	56.4	76.2	84.7	
tube passes	1	1	1	1	
P	0.284	0.228	0.218	0.216	
R	0.725	2.848	3.617	3.803	
correction factor LMTD	0.90	0.78	0.75	0.75	from 'Brown'
Delta T	65.8	44.0	57.1	63.5	
A (m^2)	8.73	28.37	7.55	1.55	
di (m)	0.016	0.016	0.016	0.016	
do (m)	0.020	0.020	0.020	0.020	
L (m)	2.5	2.5	2.5	2.5	
tube wall material	carbon steel	carbon steel	carbon steel	carbon steel	
A bare tube (m2)	0.16	0.16	0.16	0.16	
number of bare tubes	19	415	91	18	
fan power (kW)	1.07	3.00	0.77	0.16	from 'Glass'
Pressure tubes (bar)	13.0	1.3	1.3	1.3	

Appendix E4. List of utilities

Equipment number	Steam LP		Steam MP		Electricity (W)
	(W)	(kg/s)	(W)	(kg/s)	
H13	-		7.25E+06	3.36E+00	-
H15	-		-		2.69E+04
H18	-		-		1.07E+03
H22	-		1.31E+05	6.00E-02	-
H23	-		-		1.00E+03
H26	-		-		3.00E+03
H29	-		1.84E+05	? 1.19E+00	-
H30	-		-		4.00E+02
H33	-		-		1.60E+02
H34	-		-		7.70E+02
H8	5.91E+06	2.62E+00	-		-
H9	-		-		7.46E+04
P1	-		-	116	1.16E+02
P2	-		-		5.08E+03
P3	-		-		9.09E+03
P4	-		-		4.49E+02
P6	-		-		2.94E+04
P14	-		-		7.03E+02
P20	-		-		2.90E+03
P27	-		-	316	3.16E+02
P35	-		-		5.45E+01
P36	-		-		8.50E+00
Total	5.91E+06	2.62E+00	7.56E+06	4.61E+00	1.56E+05

Appendix F.1 SPECIFICATION FORM TOWERS

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO nr. : 3206

Date : 5/1/98
Designers :
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER : T7

General Properties

Function = fractionator

Tower Type = plate type column

Tray Type = sieve plate

Number of trays
- theoretical = 25
- real = 32
- feed tray(real) = 20
Tray material = AISI 405

Tower height [m] = 16.56
Tower material = carbon steel

Heating = reboiler

Operating conditions

	Feed		**Top**		**Bottom**		**Reflux**	
Temp. [°C]	:70.9		:64.5		:130.0		:64.5	
Pressure [bar]	:1.013		:1.013		:1.313		:1.013	
Density [kg/m^3]	:4.8		:748.8		:786.8		:748.6	
Mass flow[kg/s]	:8.99		:5.79		:3.18		:1.26	
Composition	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**
Methanol		0.6489		0.9995		0.0001		0.9995
PO		0.0002		0.0003		0		0.0003
H2O		0.0002		0.0002		0.0002		0.0002
MP2		0.3154				0.8914		
MDP		0.0040				0.0113		
MTP		0				0.0001		
1,2-Propanediol		0.0001				0.0004		
MP1		0.0329				0.0932		
natriummethylaa		0.0017				0.0033		
Dipropylene Gly		0				0		
>MTP		0				0		

Rectifying Section:

Section diameter [m] = 2.8
Number of trays (real) = 23
Tray spacing [m] = 0.45

Plate design:
Active tray area [m^2] = 4.68
Weir length [m] = 2.10
Weir height [mm] = 45
Number of holes = 17875
Hole diameter[mm] = 5
Plate thickness [mm] = 5
Hole pitch [mm] = 16.2

Stripping Section:

Section diameter [m] = 2.8
Number of trays (real) = 9
Tray spacing [m] = 0.45

Plate design:
Active tray area [m^2] = 4.68
Weir length [m] = 2.10
Weir height [mm] = 45
Number of holes = 17875
Hole diameter[mm] = 5
Plate thickness [mm] = 5
Hole pitch [mm] = 16.2

Appendix F.1 SPECIFICATION FORM TOWERS

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO nr. : 3206

Date : 5/1/98
Designers :
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER : T12

General Properties

Function = **fractionator**

Tower Type = **plate type column**

Tray Type = **sieve plate**

Number of trays
- theoretical = **64**
- real = **80**
- feed tray(real) = **38**
Tray material = **AISI 405**

Tower height [m] = **48.53**
Tower material = **carbon steel**

Heating = **reboiler**

Operating conditions

	Feed	Top	Bottom	Reflux
Temp. [°C]	:130.0	:128.7	:154.5	:128.7
Pressure [bar]	:1.313	:1.313	:1.963	:1.313
Density [kg/m^3]	:786.8	:778.9	:833.8	:778.9
Mass flow[kg/s]	:3.18	:2.81	:0.37	:13.86

Composition	mol%	wt%	mol%	wt%	mol%	wt%	mol%	wt%
Methanol		0.0001		0.0001		0		0.0001
PO		0		0		0		0
H2O		0.0002		0.0002		0		0.0002
MP2		0.8914		0.9992		0.0753		0.9992
MDP		0.0113		0		0.0970		0
MTP		0.0001		0		0.0005		0
1,2-Propanediol		0.0004		0		0.0031		0
MP1		0.0932		0.0005		0.7952		0.0005
natriummethylaa		0.0033		0		0.0284		0
Dipropylene Gly		0		0		0.0005		0
>MTP		0		0		0		0

Rectifying Section:		**Stripping Section:**		
			top	bottom
Section diameter [m]	3.00	Section diameter [m]	3.00	6.07
Number of trays (real)	45	Number of trays (real)	24	11
Tray spacing [m]	0.5	Tray spacing [m]	0.5	0.7
Plate design:		Plate design:		
Active tray area [m^2]	5.37	Active tray area [m^2]	5.37	21.99
Weir length [m]	2.25	Weir length [m]	2.25	4.55
Weir height [mm]	45	Weir height [mm]	45	50
Number of holes	23256	Number of holes	27339	140011
Hole diameter[mm]	5	Hole diameter[mm]	5	5
Plate thickness [mm]	5	Plate thickness [mm]	5	5
Hole pitch [mm]	15.3	Hole pitch [mm]	14.1	13.0

Appendix F.1 SPECIFICATION FORM TOWERS

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO nr. : 3206

Date : 5/1/98
Designers :
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER : T21

General Properties

Function = fractionator

Tower Type = plate type column

Tray Type = sieve plate

Number of trays
- theoretical = 27
- real = 35
- feed tray(real) = 15
Tray material = AISI 405

Tower height [m] = 22.14
Tower material = carbon steel

Heating = reboiler

Operating conditions

	Feed		Top		Bottom		Reflux	
Temp. [°C]	:149.1		:129.8		:200.8		:129.8	
Pressure [bar]	:1.013		:1.013		:1.298		:1.013	
Density [kg/m³]	:3.7		:854.5		:765.5		:854.54	
Mass flow[kg/s]	:2.04		:1.44		:0.59		:3.29	
Composition	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**
Methanol		0		0		0		0
PO		0.0001		0.0001		0		0.0001
H2O		0		0		0		0
MP2		0.0871		0.1228		0		0.1228
MDP		0.2673		0.0071		0.8997		0.0071
MTP		0.0228		0		0.0783		0
1,2-Propanediol		0.0001		0		0.0002		0
MP1		0.6164		0.8700		0.0005		0.8700
natriummethylaa		0.0052		0		0.0177		0
Dipropylene Gly		0.0010		0		0.0034		0
>MTP		0		0		0		0

Rectifying Section:

Section diameter [m] = 1.30
Number of trays (real) = 17
Tray spacing [m] = 0.55

Plate design:
Active tray area [m^2] = 1.062
Weir length [m] = 0.936
Weir height [mm] = 45
Number of holes = 8112
Hole diameter[mm] = 5
Plate thickness [mm] = 5
Hole pitch [mm] = 10..8

Stripping Section:

Section diameter [m] = 0.85
Number of trays (real) = 18
Tray spacing [m] = 0.55

Plate design:
Active tray area [m^2] = 0.431
Weir length [m] = 0.638
Weir height [mm] = 45
Number of holes = 2636
Hole diameter[mm] = 5
Plate thickness [mm] = 5
Hole pitch [mm] = 11.2

Appendix F.1 SPECIFICATION FORM TOWERS

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO nr. : 3206

Date : 5/1/98
Designers :
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER : T28

General Properties

Function = **fractionator**

Tower Type = **plate type column, with stripping section divided into two parts with different diameters**

Tray Type = **sieve plate**

Number of trays
- theoretical = **9**
- real = **12**
- feed tray(real) = **6**
Tray material = **AISI 405**

Tower height [m] = **6.90**
Tower material = **carbon steel**

Heating = **reboiler**

Operating conditions

	Feed		**Top**		**Bottom**		**Reflux**	
Temp. [°C]	:200.8		:197.14		:229.8		:197.14	
Pressure [bar]	:1.298		:1.298		:1.406		:1.298	
Density [kg/m^3]	:765.0		:759.1		:785.6		:759.1	
Mass flow[kg/s]	:0.59		:0.50		:0.10		:0.08	
Composition	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**
Methanol		0		0		0		0
PO		0		0		0		0
H2O		0		0		0		0
MP2		0		0		0		0
MDP		0.8997		0.9912		0.4367		0.9912
MTP		0.0783		0.0070		0.4398		0.0070
1,2-Propanediol		0.0002		0.0002		0		0.0002
MP1		0.0005		0.0006		0		0.0006
natriummethylaa		0.0177		0		0.1079		0
Dipropylene Gly		0.0043		0.0010		0.0156		0.0010
>MTP		0		0		0		0

Rectifying Section:

Section diameter [m] = 0.54
Number of trays (real) = 5
Tray spacing [m] = 0.50

Plate design:
Active tray area [m^2] = 0.174
Weir length [m] = 0.405
Weir height [mm] = 45
Number of holes = 709
Hole diameter[mm] = 5
Plate thickness [mm] = 5
Hole pitch [mm] = 12.8

Stripping Section:

Section diameter [m] = 0.54
Number of trays (real) = 7
Tray spacing [m] = 0.50

Plate design:
Active tray area [m^2] = 0.174
Weir length [m] = 0.405
Weir height [mm] = 45
Number of holes = 709
Hole diameter[mm] = 5
Plate thickness [mm] = 5
Hole pitch [mm] = 12.8

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date:5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H8

Number in series : 1
Number in parallel : 1

GENERAL PROPERTIES

Type :
- ~~heat exchanger~~
- ~~cooler~~
- ~~condenser~~
- evaporator

Type of heat exchanger :
- fixed tube sheet
- ~~floating head~~
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~

Position :
- horizontal
- ~~vertical~~

Capacity	: 5906	[kW]	(berekend)
Heat transfer area	: 169.7	[m^2]	(berekend)
Overall heat transfer coefficient	: 1000	[$W/m^2.K$]	(globaal)
Logarithmic temperature difference (LMTD)	: 34.8	[°C]	
Number of tube passes	: 2		
Number of shell passes	: 1		
Correctionfactor LMTD (> 0.75)	: 1		
Corrected LMTD	: 34.8	[°C]	

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		steam LP	MP2, MP1
Mass flow	[kg/s]	2.62	14.54
Mass flow to			
- evaporate	[kg/s]	-	14.54
- condensate	[kg/s	2.62	-
Mean heat capacity	[kJ/kg.°C]	2.21	2.66
Heat of evaporation	[kJ/kg]	2131.8	406.2
Temperature IN	[°C]	200	130
Temperature OUT	[°C]	144	130
Pressure	[bar]	4	1.3
Material		AISI 304	AISI 304

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date:5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H9

Number in series: 1
Number in parallel:

GENERAL PROPERTIES

Type:	: - ~~heat exchanger~~ - ~~cooler~~ - condenser - ~~evaporator~~
Type of heat exchanger	: - ~~fixed tube sheet~~ - ~~floating head~~ - ~~hairpin~~ - ~~double pipe~~ - ~~plate heat exchanger~~ - air cooler (finned tubes)
Position	: - horizontal - ~~vertical~~

Capacity	: 7906	[kW]	(calculated)
Heat transfer area	: 532.7	[m^2]	(calculated)
Overall heat transfer coefficient	: 425	[W/m^2.K]	(global)
Logarithmic temperature difference (LMTD)	: 34.9	[°C]	
Number of tube passes	: 1		
Number of shell passes	:		
Correctionfactor LMTD (> 0.75)	: 1		
Corrected LMTD	: 34.9	[°C]	

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		air	MeOH
Mass flow	[kg/s]	653.6	7.18
Mass flow to			
- evaporate	[kg/s]	-	-
- condensate	[kg/s]	-	7.18
Mean heat capacity	[kJ/kg.°C]	1.008	2.82
Heat of evaporation	[kJ/kg]	-	1011.1
Temperature IN	[°C]	23	65
Temperature OUT	[°C]	35	65
Pressure	[bar]	1.0	1.0
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H13		**Number in series :** 1 **Number in parallel :** 1	
GENERAL PROPERTIES			
Type	: - ~~heat exchanger~~ - ~~cooler~~ - ~~condenser~~ - evaporator		
Type of heat exchanger	: - ~~fixed tube sheet~~ - floating head - ~~hairpin~~ - ~~double pipe~~ - ~~plate heat exchanger~~		
Position	: - horizontal - ~~vertical~~		
Capacity	: 7246	[kW]	(berekend)
Heat transfer area	: 82.27	[m^2]	(berekend)
Overall heat transfer coefficient	: 900	[W/m^2.K]	(globaal)
Logarithmic temperature difference (LMTD)	: 97.9	[°C]	
Number of tube passes	: 2		
Number of shell passes	: 1		
Correctionfactor LMTD (> 0.75)	: 1		
Corrected LMTD	: 97.9	[°C]	

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		steam MP	MP1
Mass flow	**[kg/s]**	3.36	121.41
Mass flow to			
- evaporate	**[kg/s]**	-	121.41
- condensate	**[kg/s]**	3.36	-
Mean heat capacity	**[kJ/kg.°C]**	2.21	2.66
Heat of evaporation	**[kJ/kg]**	1906.7	59.7
Temperature IN	**[°C]**	320	155
Temperature OUT	**[°C]**	207	155
Pressure	**[bar]**	18	1.9
Material		AISI 304	AISI 304

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H15

Number in series : /
Number in parallel :

GENERAL PROPERTIES

Type :
- ~~heat exchanger~~
- ~~cooler~~
- condenser
- ~~evaporator~~

Type of heat exchanger :
- ~~fixed tube sheet~~
- ~~floating head~~
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~
- air cooler (finned tubes)

Position :
- horizontal
- ~~vertical~~

Capacity	: 7233	[kW]	(berekend)
Heat transfer area	: 191.26	[m^2]	(berekend)
Overall heat transfer coefficient	: 425	[$W/m^2.K$]	(globaal)
Logarithmic temperature difference (LMTD)	: 89.0	[°C]	
Number of tube passes	: 1		
Number of shell passes	:		
Correctionfactor LMTD (> 0.75)	: 1		
Corrected LMTD	: 89.0	[°C]	

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		air	MP2
Mass flow	**[kg/s]**	224.24	16.70
Mass flow to			
- evaporate	**[kg/s]**	-	-
- condensate	**[kg/s]**	-	16.70
Mean heat capacity	**[kJ/kg.°C]**	1.008	2.66
Heat of evaporation	**[kJ/kg]**	-	433.1
Temperature IN	**[°C]**	23	129
Temperature OUT	**[°C]**	55	129
Pressure	**[bar]**	1.0	1.3
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date:5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H18

Number in series : 1
Number in parallel :

GENERAL PROPERTIES

Type	: - ~~heat exchanger~~ - cooler - ~~condenser~~ - ~~evaporator~~
Type of heat exchanger	: - ~~fixed tube sheet~~ - ~~floating head~~ - ~~hairpin~~ - ~~double pipe~~ - ~~plate heat exchanger~~ - air cooler (finned tubes)
Position	: - horizontal - ~~vertical~~

Capacity	: 230	[kW]	(berekend)
Heat transfer area	: 8.73	[m^2]	(berekend)
Overall heat transfer coefficient	: 400	[$W/m^2.K$]	(globaal)
Logarithmic temperature difference (LMTD)	: 73.1	[°C]	
Number of tube passes	: 1		
Number of shell passes	:		
Correctionfactor LMTD (> 0.75)	: 0.9		
Corrected LMTD	: 65.8	[°C]	

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		air	MP1
Mass flow	[kg/s]	8.27	5.81
Mass flow to			
- evaporate	[kg/s]	-	-
- condensate	[kg/s]	-	-
Mean heat capacity	[kJ/kg.°C]	1.008	2.61
Heat of evaporation	[kJ/kg]	-	-
Temperature IN	[°C]	23	120
Temperature OUT	[°C]	51	100
Pressure	[bar]	1.0	13.0
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H22	**Number in series : 1** **Number in parallel : 1**

GENERAL PROPERTIES

Type	: - ~~heat exchanger~~ - ~~cooler~~ - ~~condenser~~ - evaporator		
Type of heat exchanger	: - ~~fixed tube sheet~~ - floating head - ~~hairpin~~ - ~~double pipe~~ - ~~plate heat exchanger~~		
Position	: - horizontal - ~~vertical~~		
Capacity	: 131	[kW]	(berekend)
Heat transfer area	: 4.29	[m^2]	(berekend)
Overall heat transfer coefficient	: 800	[$W/m^2.K$]	(globaal)
Logarithmic temperature difference (LMTD)	: 38.0	[°C]	
Number of tube passes	: 2		
Number of shell passes	: 1		
Correctionfactor LMTD (> 0.75)	: 1		
Corrected LMTD	: 38.0	[°C]	

OPERATING CONDITIONS

		Shell-side	**Tube-side**
Medium		steam MP	MDP, MTP
Mass flow	**[kg/s]**	0.06	0.41
Mass flow to			
- evaporate	**[kg/s]**	-	0.41
- condensate	**[kg/s]**	0.06	-
Mean heat capacity	**[kJ/kg.°C]**	2.26	2.70
Heat of evaporation	**[kJ/kg]**	1906.7	319.5
Temperature IN	**[°C]**	320	201
Temperature OUT	**[°C]**	207	201
Pressure	**[bar]**	18	1.3
Material		AISI 304	AISI 304

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date:5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H23

Number in series : 1
Number in parallel :

GENERAL PROPERTIES

Type : - ~~heat exchanger~~
- ~~cooler~~
- condenser
- ~~evaporator~~

Type of heat exchanger : - ~~fixed tube sheet~~
- ~~floating head~~
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~
- air cooler (finned tubes)

Position : - horizontal
- ~~vertical~~

Capacity : 277 [kW] (berekend)
Heat transfer area : 7.26 [m^2] (berekend)
Overall heat transfer coefficient : 425 [$W/m^2.K$] (globaal)
Logarithmic temperature difference (LMTD): 89.9 [°C]

Number of tube passes : 1
Number of shell passes :

Correctionfactor LMTD (> 0.75) : 1
Corrected LMTD : 89.9 [°C]

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		air	MeOH
Mass flow	[kg/s]	8.59	4.74
Mass flow to			
- evaporate	[kg/s]	-	-
- condensate	[kg/s]	-	4.74
Mean heat capacity	[kJ/kg.°C]	1.008	2.66
Heat of evaporation	[kJ/kg]	-	58.4
Temperature IN	[°C]	23	130
Temperature OUT	[°C]	55	130
Pressure	[bar]	1.0	1.0
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:

M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H26

Number in series : 1
Number in parallel :

GENERAL PROPERTIES

Type : - ~~heat exchanger~~
- cooler
- ~~condenser~~
- ~~evaporator~~

Type of heat exchanger : - ~~fixed tube sheet~~
- ~~floating head~~
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~
- air cooler (finned tubes)

Position : - horizontal
- ~~vertical~~

Capacity : 499 [kW]
Heat transfer area : 28.37 [m^2]
Overall heat transfer coefficient : 400 [W/m^2.K]
Logarithmic temperature difference (LMTD): 56.4 [°C]

Number of tube passes : 1
Number of shell passes :

Correctionfactor LMTD (> 0.75) : 0.78
Corrected LMTD : 44.0 [°C]

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		air	MP2
Mass flow	**[kg/s]**	20.52	2.81
Mass flow to			
- evaporate	**[kg/s]**	-	-
- condensate	**[kg/s]**	-	-
Mean heat capacity	**[kJ/kg.°C]**	1.008	2.58
Heat of evaporation	**[kJ/kg]**	-	-
Temperature IN	**[°C]**	23	129
Temperature OUT	**[°C]**	47	60
Pressure	**[bar]**	1.0	1.3
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H29

Number in series : 1
Number in parallel :

GENERAL PROPERTIES

Type : - ~~heat exchanger~~
- ~~cooler~~
- ~~condenser~~
- evaporator

Type of heat exchanger : - ~~fixed tube sheet~~
- floating head
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~

Position : - horizontal
- ~~vertical~~

Capacity : 184 [kW] (berekend)
Heat transfer area : 5.65 [m^2] (berekend)
Overall heat transfer coefficient : 700 [$W/m^2.K$] (globaal)
Logarithmic temperature difference (LMTD): 46.5 [°C]

Number of tube passes : 2
Number of shell passes : 1

Correctionfactor LMTD (> 0.75) : 1
Corrected LMTD : 46.5 [°C]

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		steam MP	MTP
Mass flow	[kg/s]	1.19	0.51
Mass flow to			
- evaporate	[kg/s]	-	0.51
- condensate	[kg/s]	-	-
Mean heat capacity	[kJ/kg.°C]	2.26	2.59
Heat of evaporation	[kJ/kg]	-	360.8
Temperature IN	[°C]	320	230
Temperature OUT	[°C]	250	230
Pressure	[bar]	18	1.4
Material		AISI 304	AISI 304

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H30

Number in series : 1
Number in parallel :

GENERAL PROPERTIES

Type : - ~~heat exchanger~~
- ~~cooler~~
- condenser
- ~~evaporator~~

Type of heat exchanger : - ~~fixed tube sheet~~
- ~~floating head~~
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~
- air cooler (finned tubes)

Position : - horizontal
- ~~vertical~~

Capacity : 181 [kW] (berekend)
Heat transfer area : 2.91 [m^2] (berekend)
Overall heat transfer coefficient : 425 [W/m^2.K] (globaal)
Logarithmic temperature difference (LMTD): 146.6 [°C]

Number of tube passes : 1
Number of shell passes :

Correctionfactor LMTD (> 0.75) : 1
Corrected LMTD : 146.6 [°C]

OPERATING CONDITIONS

		Shell-side	Tube-side
Medium		air	MDP
Mass flow	[kg/s]	3.45	0.58
Mass flow to			
- evaporate	[kg/s]	-	-
- condensate	[kg/s]	-	0.58
Mean heat capacity	[kJ/kg.°C]	1.008	2.73
Heat of evaporation	[kJ/kg]	-	
Temperature IN	[°C]	23	197
Temperature OUT	[°C]	35	197
Pressure	[bar]	1.0	1.3
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H33

Number in series :
Number in parallel :

GENERAL PROPERTIES

Type : - heat exchanger
- cooler
- condenser
- evaporator

Type of heat exchanger : - fixed tube sheet
- floating head
- hairpin
- double pipe
- plate heat exchanger
- air cooler (finned tubes)

Position : - horizontal
- vertical

Capacity : 39 [kW]
Heat transfer area : 1.55 [m^2]
Overall heat transfer coefficient : 400 [$W/m^2.K$]
Logarithmic temperature difference (LMTD): 84.7 [°C]

Number of tube passes : 1
Number of shell passes :

Correctionfactor LMTD (> 0.75) : 0.75
Corrected LMTD : 63.5 [°C]

OPERATING CONDITIONS

		Shell-side	**Tube-side**
Medium		air	MTP
Mass flow	**[kg/s]**	0.87	0.10
Mass flow to			
- evaporate	**[kg/s]**	-	-
- condensate	**[kg/s]**	-	-
Mean heat capacity	**[kJ/kg.°C]**	1.008	2.37
Heat of evaporation	**[kJ/kg]**	-	-
Temperature IN	**[°C]**	23	230
Temperature OUT	**[°C]**	68	60
Pressure	**[bar]**	1.0	1.3
Material			carbon steel

Appendix F2 Specification forms heat exchangers

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. :3206

Date: 5-1-1998
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: H34

Number in series : 1
Number in parallel :

GENERAL PROPERTIES

Type : - ~~heat exchanger~~
- cooler
- ~~condenser~~
- ~~evaporator~~

Type of heat exchanger : - ~~fixed tube sheet~~
- ~~floating head~~
- ~~hairpin~~
- ~~double pipe~~
- ~~plate heat exchanger~~
- air cooler (finned tubes)

Position : - horizontal
- ~~vertical~~

Capacity : 173 [kW]
Heat transfer area : 7.55 [m^2]
Overall heat transfer coefficient : 400 [W/m^2.K]
Logarithmic temperature difference (LMTD): 76.2 [°C]

Number of tube passes : 1
Number of shell passes :

Correctionfactor LMTD (> 0.75) : 0.75
Corrected LMTD : 57.1 [°C]

OPERATING CONDITIONS

		Shell-side	**Tube-side**
Medium		air	MDP
Mass flow	**[kg/s]**	4.52	0.50
Mass flow to			
- evaporate	**[kg/s]**	-	-
- condensate	**[kg/s]**	-	-
Mean heat capacity	**[kJ/kg.°C]**	1.008	2.53
Heat of evaporation	**[kJ/kg]**	-	-
Temperature IN	**[°C]**	23	197
Temperature OUT	**[°C]**	61	60
Pressure	**[bar]**	1.0	1.3
Material			carbon steel

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P1		
Type:	rotary pump	
Fluid:	sodiummethylate	
Temperature (T):	20	[°C]
Density (ρ):	937.8	[kg/m^3]
Viscosity (μ):	0.63	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	4.436e-5	[m3/s]
Inlet pressure (P_z):	1.3	[bar]
Outlet pressure (P_p):	27.5	[bar]
Theoretical power ($=\phi_v(P_p-P_z)$):	0.116	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	0.166	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P2		
Type:	rotary pump	
Fluid:	MeOH	
Temperature (T):	20	[°C]
Density (ρ):	803.5	[kg/m^3]
Viscosity (μ):	0.69	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	1.356e-3	[m3/s]
Inlet pressure (P_z):	1.3	[bar]
Outlet pressure (P_p):	27.5	[bar]
Theoretical power ($=\phi_v(P_p-P_z)$):	3.552	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	5.075	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P3		
Type:	rotary pump	
Fluid:	PO	
Temperature (T):	20	[°C]
Density (ρ):	828.2	[kg/m^3]
Viscosity (μ):	0.31	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	2.427e-3	[m3/s]
Inlet pressure (P_z):	1.3	[bar]
Outlet pressure (P_p):	27.5	[bar]
Theoretical power ($=\phi_v(P_p-P_z)$):	6.359	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	9.084	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P4		
Type:	rotary pump	
Fluid:	PO	
Temperature (T):	20	[°C]
Density (ρ):	828.2	[kg/m^3]
Viscosity (μ):	0.31	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	2.683e-4	[m3/s]
Inlet pressure (P_z):	1.3	[bar]
Outlet pressure (P_p):	13.0	[bar]
Theoretical power (=$\phi_v(P_p-P_z)$):	0.314	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	0.448	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P6		
Type:	rotary pump	
Fluid:	MeOH	
Temperature (T):	64.5	[°C]
Density (ρ):	748.6	[kg/m^3]
Viscosity (μ):	0.35	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	7.766e-3	[m3/s]
Inlet pressure (P_z):	1.0	[bar]
Outlet pressure (P_p):	27.5	[bar]
Theoretical power ($=\phi_v(P_p-P_z)$):	20.570	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	29.385	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P14		
Type: Fluid: Temperature (T): Density (ρ): Viscosity (μ): Vapour pressure (Pd):	rotary pump mainly MP1 155 833.8 0.24 -	 [°C] [kg/m^3] [mPa.s] [bar]
Capacity (ϕ_v): Inlet pressure (P_z): Outlet pressure (P_p): Theoretical power ($=\phi_v(P_p-P_z)$): Pump efficiency (η): Axis power:	4.454e-4 1.9 13.0 0.491 0.70 0.702	[m3/s] [bar] [bar] [kW] [-] [kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P20		
Type:	rotary pump	
Fluid:	MP1	
Temperature (T):	130	[°C]
Density (ρ):	854.5	[kg/m^3]
Viscosity (μ):	0.28	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	1.689e-3	[m3/s]
Inlet pressure (P_z):	1.0	[bar]
Outlet pressure (P_p):	13.0	[bar]
Theoretical power (=$\phi_v(P_p-P_z)$):	2.024	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	2.892	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P27		
Type:	rotary pump	
Fluid:	MP-2	
Temperature (T):	60	[°C]
Density (ρ):	872.9	[kg/m^3]
Viscosity (μ):	0.62	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	3.221e-4	[m3/s]
Inlet pressure (P_z):	1.3	[bar]
Outlet pressure (P_p):	2.0	[bar]
Theoretical power ($=\phi_v(P_p-P_z)$):	0.022	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	0.032	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

EQUIPMENT NUMBER: P35		
Type:	rotary pump	
Fluid:	MDP	
Temperature (T):	60	[°C]
Density (ρ):	914.3	[kg/m^3]
Viscosity (μ):	3.2	[mPa.s]
Vapour pressure (Pd):	-	[bar]
Capacity (ϕ_v):	5.186e-4	[m3/s]
Inlet pressure (P_z):	1.3	[bar]
Outlet pressure (P_p):	2.0	[bar]
Theoretical power ($=\phi_v(P_p-P_z)$):	0.036	[kW]
Pump efficiency (η):	0.70	[-]
Axis power:	0.0052	[kW]
Construction material:	carbon steel	

Appendix F3. Specification forms pumps

Technische Universiteit Delft
Vakgroep Chemische Procestechnologie

FVO Nr. 3206

Date: 5-1-98
Designers:
M.G. van den Eijnden
J.C. IJsebaert
B.R. Regenbogen
F.A.M. Wieland

SPECIFICATION FORM PUMP

EQUIPMENT NUMBER: P36		
Type: Fluid: Temperature (T): Density (ρ): Viscosity (μ): Vapour pressure (Pd):	rotary pump MTP 60 979.1 1.9 -	 [°C] [kg/m^3] [mPa.s] [bar]
Capacity (ϕ_v): Inlet pressure (P_z): Outlet pressure (P_p): Theoretical power ($=\phi_v(P_p-P_z)$): Pump efficiency (η): Axis power:	9.583e-5 1.4 2.0 0.006 0.70 0.008	[m3/s] [bar] [bar] [kW] [-] [kW]
Construction material:	carbon steel	

Appendix G1. Equipment list reactors and distillation columns

FVO Nr. 3206

EQUIPMENT NR.	**R5**	**T7**	**T12**	**R19**
Name	reactor	distillation column	distillation column	reactor
Type	multitubular	plate column	plate column	multitubular
Pressure (abs.) [bar]	27.5	1.0-1.3	1.3-2.0	13.0
Temperature (top/bottom) [°C]	profile	65/130	129/155	profile
Volume [m^3]	7			1.2
Diameter [m]	1.94	2.80	3/ 6.07	1
Length [m]	10	15.56	48.53	10
Filling	none (homogeneous catalyst)			none (homogeneous catalyst)
Trays (+ number)		sieve plates 32 (real)	sieve plates 80 (real)	
Solid packing		-	-	
Cat. type		-	-	
Cat. shape		-	-	
Construction material	carbon steel	carbon steel	carbon steel	carbon steel
Number in				
- series	1	1	1	1
- parallel				
Other				

Appendix G1. Equipment list reactors and distillation columns

FVO Nr. 3206

EQUIPMENT NR.	T21	T28
Name	distillation column	distillation column
Type	plate column	plate column
Pressure (abs.) [bar]	1.0/1.3	1.3/1.4
Temperature (top/bottom) [°C]	130/201	197/230
Volume [m^3]		
Diameter [m]	0.85/1.3	0.54
Length [m]	22.14	6.9
Filling		
Trays	sieve plates	sieve plates
(+ number)	35 (real)	12 (real)
Solid packing	-	–
Cat. type	-	–
Cat. shape	-	–
Construction material	carbon steel	carbon steel
Number in		
- series	1	1
- parallel		
Other		

Appendix G2. Equipment list heat exchangers

FVO Nr.3206

EQUIPMENT NR.	**H8**	**H9**	**H13**	**H15**
Name **Type**	reboiler thermosyphon	condenser air cooled	reboiler thermosyphon	condenser air cooled
Medium **- tubes** **- shell**	MP-2,MP-1 cond. steam LP	MeOH air	MP-1 cond. steam MP	MP-2 air
Capacity **Heat duty** **[kW]**	5906	7906	7246	7233
Heat transfer area **[m^2]**	169.73	532.7	82.27	191.26
Number **- series** **- parallel**	1	1	1	1
Pressure (abs) **- tubes** **- shell** **[bar]**	1.3 4.0	1.0 1.0	1.9 18.0	1.3 1.0
Temperature **IN/OUT** **- tubes** **- shell** **[°C]**	130/130 200/144	65/65 23/35	155/155 320/207	129/129 23/55
Construction material	AISI 304	carbon steel	AISI 304	carbon steel
Other				

Appendix G2. Equipment list heat exchangers

FVO Nr.3206

EQUIPMENT NR.	**H18**	**H22**	**H23**	**H26**
Name **Type**	cooler air cooler	reboiler thermosyphon	condenser air cooled	cooler air cooler
Medium **- tubes** **- shell**	 mainly MP-1 air	 MDP, MTP cond. steam MP	 MP-1 air	 MP-2 air
Capacity Heat duty [kW]	230	131	277	499
Heat transfer area [m^2]	8.73	4.29	7.26	28.37
Number **- series** **- parallel**	1	1	1	1
Pressure (abs) **- tubes** **- shell** **[bar]**	 13.0 1.0	 1.3 18.0	 1.0 1.0	 1.3 1.0
Temperature IN/OUT **- tubes** **- shell** **[°C]**	 120/100 23/51	 201/201 320/207	 130/130 23/55	 129/60 23/47
Construction material	carbon steel	AISI 304	carbon steel	carbon steel
Other				

Appendix G2. Equipment list for heat exchangers

FVO Nr.3206

EQUIPMENT NR.	H29	H30	H33	H34
Name Type	reboiler thermosyphon	condenser air cooled	cooler air cooler	cooler air cooler
Medium - tubes - shell	 MTP steam MP	 MDP air	 mainly MTP air	 MDP air
Capacity Heat duty [kW]	184	181	39	173
Heat transfer area [m^2]	5.65	2.91	1.55	7.55
Number - series - parallel	1	1	1	1
Pressure (abs) - tubes - shell [bar]	 1.4 18.0	 1.3 1.0	 1.3 1.0	 1.3 1.0
Temperature IN/OUT - tubes - shell [°C]	 230/230 320/250	 197/197 23/75	 230/60 23/68	 197/197 23/61
Construction material	AISI 304	carbon steel	carbon steel	carbon steel
Other				

Appendix G3. Equipment list pumps

FVO Nr. 3206

EQUIPMENT NR.	P1	P2	P3	P4	P6
Name Type	pump rotary	pump rotary	pump rotary	pump rotary	pump rotary
Fluid	sodiummethylate	MeOH	PO	PO	MeOH(recycle)
Capacity [kg/s]	0.042	1.09	2.05	2.22	5.81
Density [kg/m^3]	952.7	805.3	844.3	828.2	748.6
Inlet/Outlet pressure (abs) [bar]	1.3/27.5	1.3/27.5	1.3/27.5	1.3/13.0	1.0/27.5
Temp. In/Out [°C]	20.0/21.9	20.0/21.9	20.0/22.2	20.0/21.0	64.5/66.3
Power - theory - practice [kW]	 0.116 0.166	 3.553 5.075	 6.359 9.084	 0.314 0.448	 20.570 29.385
Number - series - parallel	1	1	1	1	1
Construction material	carbon steel	carbon steel	carbon steel	carbon steel	carbon steel
Other					

Appendix G3. Equipment list pumps

FVO Nr. 3206

EQUIPMENT NR.	**P14**	**P20**	**P27**	**P35**	**P36**
Name	pump	pump	pump	pump	pump
Type	rotary	rotary	rotary	rotary	rotary
Fluid	mainly MP1	MP1	MP2	MDP	MTP
Capacity [kg/s]	0.371	1.44	2.81	0.050	0.098
Density [kg/m^3]	833.8	854.5	873.0	914.4	979.1
Inlet/Outlet pressure (abs) [bar]	1.9/13.0	1.0/13.0	1.3/2.0	1.3/2.0	1.3/2.0
Temp. In/Out [°C]	154.5/155.1	129.8/130.6	60.0/60.0	60.0/60.0	60.0/60.0
Power					
- theory	0.491	2.024	0.022	0.036	0.0056
- practice	0.702	2.892	0.032	0.052	0.0080
[kW]					
Number	1	1	1	1	1
- series					
- parallel					
Construction material	carbon steel	carbon steel	carbon steel	carbon steel	carbon steel
Other					

Appendix H.1: Equipment costs

REACTORS		
	Reactor R5	**Reactor R19**
Heat transfer area (m^2):	731.71	121.95
Material shell:	Carbon Steel	Carbon Steel
Material pipes:	Carbon Steel	Carbon Steel
Reactor cost (fl, 1995)	280560	108125
Reactor cost (fl, 1997)	**287816**	**110921**

TOWERS						
	Tower T7	**Tower T12**		**Tower T21**		**Tower T28**
Section	rect.+ stripping	rectifying+strip	stripping	rectifying	stripping	rect.+ strip
Diameter (m):	2.812	3	6.07	1.31	0.851	0.548
Column thickness (mm)	12			10	10	8
Height (m)	14.4	34.5	7.7	9.35	9.9	6
Material:	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel
Cost of the column (fl, 1995):	179000		265000	84000	66750	39300
Plate type	sieve tray	sieve tray	sieve tray	sieve tray	sieve tray	sieve tray
Plate material	AISI 405	AISI 405	AISI 405	AISI 405	AISI 405	AISI 405
Plate diameter	2.8	3	6.07	1.3	0.85	0.54
Cost of a plate per m^2 (fl):	962	940	760	1267	1500	1800
Area (m^2):	5.42	6.22	25.47	1.20	0.50	0.20
Number of plates:	32	69	11	17	18	12
Total costs of plates (fl, 1995):	166818	403429	212929	25739	13473	4363
Total tower cost (fl, 1995):	345818	403429	477929	109739	80223	43663
Total tower cost (fl, 1997):	354762	413863	490289	112577	82298	44792
Total tower cost (fl, 1997):	**354762**		**904152**		**194875**	**44792**

REBOILERS				
	Reboiler H8	**Reboiler H13**	**Reboiler H22**	**Reboiler H29**
Heat transfer area (m^2):	148.00	346.00	3.00	5.65
Material pipes:	AISI 304	AISI 304	AISI 304	AISI 304
Material shell:	AISI 304	AISI 304	AISI 304	AISI 304
Total reboiler cost (fl, 1995)	176000	316000	26000	29500
Total reboiler cost (fl, 1997)	**180552**	**324172**	**26672**	**30263**

CONDENSERS				
	Condenser H9	**Condenser H10**	**Condenser H23**	**Condenser H30**
Heat transfer area (m^2):	532.7	191.26	7.26	2.91
Heat transfer area (ft^3):	5734.12	2058.77	78.15	31.32
Material pipes:	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel
Total cooler cost ($, 1987):	45420	30461	8505	5954
Total cooler cost (fl, 1987):	92202	61837	17265	12087
Total cooler cost (fl, 1997):	**107569**	**72143**	**20143**	**14102**

AIR COOLERS				
	Cooler H18	**Cooler H26**	**Cooler H34**	**Cooler H33**
Heat transfer area (m^2):	8.73	28.37	7.55	1.55
Heat transfer area (ft^3):	93.97	305.38	81.27	16.68
Material pipes:	Carbon Steel	Carbon Steel	Carbon Steel	Carbon Steel
Total cooler cost ($, 1987):	9139	14472	8636	4657
Total cooler cost (fl, 1987):	18553	29378	17531	9455
Total cooler cost (fl, 1997):	**21645**	**34275**	**20453**	**11030**

Pumps ?

Appendix H2. Economic Evaluation Criteria

Cash-flow diagram calculations

Item	Cost (kfl/a)	Cumulative years	Cumulative cash flow (kfl/a)
designing	1,278	1	-1,278
building of plant	11,080	3	-12,358
working capital	1,854	3	-14,212

Operating costs (kfl/a)	Income (kfl/a)	Cumulative years	Cumulative cash flow (kfl/a)	
171,524	182,453	4	-3,283	1 +3
171,524	182,453	5	7,645	2
171,524	182,453	6	18,574	3
171,524	182,453	7	29,503	4
171,524	182,453	8	40,432	5
171,524	182,453	9	51,360	6
171,524	182,453	10	62,289	7
171,524	182,453	11	73,218	8
171,524	182,453	12	84,147	9
171,524	182,453	13	95,075	10
171,524	182,453	14	106,004	11
171,524	182,453	15	116,933	12
171,524	182,453	16	127,862	13
171,524	182,453	17	138,790	14
171,524	182,453	18	149,719	15 +3

(2) (1)

Rate of return calculation

ROR = ((F-C)/(C*G))*100%

F = 149,719
C = 14,212
G = 15

ROR = 63.56%

Appendix H2. Economic Evaluation Criteria

NPW and TNPW calculation

Discount rate r = 0.16

Year n	NFW (kfl)	NPW (kfl)	TNPW
1	-1,278	-1,102	-1,102
2	-6,818	-5,067	-6,169
3	-14,212	-9,105	-15,274
4	-3,283	-1,813	-17,087
5	7,645	3,640	-13,447
6	18,574	7,624	-5,824
7	29,503	10,439	4,615
8	40,432	12,333	16,948
9	51,360	13,505	30,453
10	62,289	14,120	44,573
11	73,218	14,308	58,881
12	84,147	14,176	73,057
13	95,075	13,807	86,864
14	106,004	13,271	100,136
15	116,933	12,620	112,756
16	127,862	11,896	124,652
17	138,790	11,132	135,784
18	149,719	10,352	146,136

DCFRR

The DCFRR is the discount rate at which the TNPW at the end of the plant life time equals zero. The value can be found by trial-and -error; varying the value of r.

DCFRR = 0.565