FVO Nr. 3181

Preliminary Design Project
Department of Chemical Engineering

Subject
Design of a process for the production of 
para-xylene and ortho-xylene from a mixed 
xylenes feed

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Keywords
para-Xylene, ortho-Xylene, Xylene isomerization,
Leuna Kontakt 8835, para-Xylene separation,
adsorption, crystallization.

Date assignment : 17 September 1996
Date report : 20 December 1996
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Summary

In this Preliminary Design Project (FVO) two options were examined to increase the para-xylene production for a grassroots aromatics complex, including a xylene splitter, an ortho-xylene column, a crystallization unit to separate the para-xylene and a xylene isomerization unit. First a new catalyst, the Leuna Kontakt 8835 was used. Secondly the effects of an additional adsorption unit for the para-xylene separation were examined. For this option the possible bottle necks in the process were determined. The para-xylene separation unit was handled as a black box.

The design capacity of the aromatics complex was 130,000 ton/year of fresh mixed xylenes feed. The aromatics complex can be divided in three sections; the reaction section and two separation sections, one upstream, and one downstream the reaction section. In the upstream separation section the products, para- and ortho-xylene, were separated from the reactor feed stream. In the reaction section the mixed xylenes were isomerized to near equilibrium composition. The ethylbenzene was mainly converted to benzene and ethane. A H₂/C₅ molar ratio of 3 mol/mol in the reactor was maintained. In the downstream separation section first the hydrogen and light hydrocarbons were flashed and recycled, secondly the C₇-fraction was separated from the liquid recycle stream.

The main products were para-xylene and ortho-xylene which were produced with a minimum purity of respectively 99.70 wt% and 99.00 wt%. The para-xylene production with the Leuna Kontakt 8835 catalyst amounted 71,140 ton/year and the ortho-xylene production was 32,350 ton/year. The addition of the adsorption unit allowed a 26 % increase of the fresh mixed xylenes feed to 164,000 ton/year. In this situation the production of para-xylene increased with 43 % to 101,440 ton/year and the ortho-xylene production became 30,750 ton/year. By-products were a heavy ends stream, a light ends stream rich of benzene and toluene, and a purge stream, which only has a fuel value.

Almost no bottle necks occur when an additional adsorption unit is installed. The capacities and heat duties of all units are still sufficient but the toluene concentration in the feed to the para-xylene separation unit will become too high when an adsorption unit is installed. When the para-xylene production is further increased the heat duties of the aircooler H2 and reboiler H3 will become insufficient.

A hazard and operability study (HAZOP) and a safety analysis according to Dow's Fire and Explosion Index were performed. From these studies it was concluded that because of the presence of hydrogen and hydrocarbons above their flash points special care should be taken in operating the process.

An economical analysis was made for the original design without an adsorption unit. The price of para-xylene is rather fluctuating because of the growing demand and production capacity. For the economical analysis a price of 500 $/ton was assumed. This resulted in an annual profit of $ 4,800,000. The Return On Investment and the Internal Rate of Return were respectively 12.4 % and 13 %. The Pay-Out-Time was 20 months. In conclusion it can be said that the process is profitable.
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<td>L-1</td>
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Introduction

1. Introduction

para-Xylene is a base chemical. It is mainly used to produce polyester fibers, resins and films. para-Xylene can be obtained from a mixed xylenes stream originating from a refinery. The mixed xylenes stream consists mainly of para-xylene, meta-xylene, ortho-xylene and ethylbenzene. Most of the para-xylene in the feed is separated from the other compounds. Traditionally this is done by crystallization. The crystallization filtrate is fed to a reactor where para-xylene is formed by isomerization of the xylenes. The ethylbenzene is dealkylated to benzene and ethane, or isomerized to xylenes.

Over the last ten years the para-xylene consumption has grown steadily worldwide. The para-xylene consumption increased from 4.2 million tonnes in 1984 to 9.0 million tonnes in 1993. The forecasts are that this growth will maintain in the years to come. To keep up with this rising demand an increase of the production capacity from 10.6 million ton/year in 1993 to about 16.4 million ton/year in 2000 will be necessary. For example Exxon is going to triple the para-xylene production capacity in the Botlek by 1998.

The para-xylene price is rather fluctuating because of the growing demand for para-xylene and the growing production capacity.

Strategies to increase para-xylene capacity can be divided in three categories:

- Short term strategies
  - Increase operation rates, replace catalysts
- Medium term strategies
  - Revamp process units to higher capacity and convert existing units to new services
- Long term strategies
  - Build new aromatic complexes and replace crystallizers by adsorption units

In this Preliminary Design Project (FVO), a short term strategy as well as a long term strategy will be examined for Raytheon Engineers & Constructors, Den Haag.

First a short term strategy will be examined. A para-xylene isomerization plant will be designed with a new catalyst, the Leuna Kontakt 8835, which is capable to reach a high para-xylene production. This high production can be obtained due to the near equilibrium composition of the isomerized xylenes and due to a high ethylbenzene conversion per reactor pass.

Secondly a long term strategy will be examined. The effect of the installation of an adsorption unit, in addition to the crystallization unit, on the existing plant will be examined. Possible bottle necks in the process will be determined, while the volumetric flow to the reactor is maintained.
2. **Basis of design**

2.1 **Description of process**

The feed streams for the process are a mixed xylenes feed which is obtained from a refinery, and a hydrogen stream which is obtained from a platformer. A short description of the process is given below:

The mixed xylenes feed is first fed to a distillation column where a part of the ortho-xylene and all the heavy ends are separated from the lighter products. The top stream of this column is fed to the para-xylene separation unit. The bottom stream of the xylene splitter is fed to another distillation column where the ortho-xylene is purified.

The para-xylene separation unit separates the para-xylene from the top stream of the xylene splitter, and the filtrate is fed to the reactor section. Two situations will be examined for the para-xylene separation. First a crystallization unit will be used as para-xylene separation unit. Second the para-xylene separation unit will be a combination of an adsorption unit and a crystallization unit. In both situations the para-xylene separation unit will be handled as a black box.

The filtrate of the para-xylene separator is fed to the isomerization reactor. In this reactor xylene isomerization and ethylbenzene conversion take place in presence of hydrogen. The catalyst used in this reactor is the Leuna Kontakt 8835.

Downstream of the reactor a gas/liquid separator separates the hydrogen and light hydrocarbons from the liquid stream. The C7 products of the liquid stream are removed by distillation and the xylene-recycle is clay treated to remove small amounts of impurities.

The bottom stream of the xylene splitter is fed to the ortho-xylene column, where the ortho-xylene is purified. The bottom stream of this column is the C9 fraction.

In figure 2.1 a schematic representation of the process is given.

![Schematic representation of the process](image)
2.2 Initial criteria

In appendix G a Table with the most important physical properties of all components which occur in this process is presented. In the following paragraphs the specifications of the feed and product streams, the battery limit, the catalyst and the reactor conditions and performance will be given.

2.2.1 Feed streams

The design capacity of the process is 130,000 ton/year of fresh mixed xylenes feed. The yearly capacity is based on 8000 operating hours per year. The composition of mixed xylenes feed is given in Table 2.1.

Table 2.1 Composition of fresh mixed xylenes

<table>
<thead>
<tr>
<th>Component</th>
<th>Composition [wt%]</th>
<th>Flowrate [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toluene</td>
<td>1.0</td>
<td>162.5</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>16.0</td>
<td>2,600.0</td>
</tr>
<tr>
<td>para-Xylene</td>
<td>21.0</td>
<td>3,412.5</td>
</tr>
<tr>
<td>meta-Xylene</td>
<td>52.0</td>
<td>8,450.0</td>
</tr>
<tr>
<td>ortho-Xylene</td>
<td>10.0</td>
<td>1,625.0</td>
</tr>
<tr>
<td>Total</td>
<td>100.0</td>
<td>16,250.0</td>
</tr>
</tbody>
</table>

For this design capacity and a H2/C4 molar ratio of 3 mol/mol in the reactor a make-up hydrogen stream of 904.1 kg/h is needed. The composition of this stream is given in Table 2.2, Nelson (1958).

Table 2.2 Composition of make-up hydrogen

<table>
<thead>
<tr>
<th>Component</th>
<th>Composition [vol%]</th>
<th>Flowrate [kg/h]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>80.8</td>
<td>183.0</td>
</tr>
<tr>
<td>Methane</td>
<td>5.0</td>
<td>90.8</td>
</tr>
<tr>
<td>Ethane</td>
<td>4.9</td>
<td>166.9</td>
</tr>
<tr>
<td>Propane</td>
<td>9.3</td>
<td>463.4</td>
</tr>
<tr>
<td>Total</td>
<td>100.0</td>
<td>904.1</td>
</tr>
</tbody>
</table>

2.2.2 Products

The main products of the process are para-xylene and ortho-xylene. The specifications of these products can be found in Table 2.3.
Table 2.3 Specifications of the main products

<table>
<thead>
<tr>
<th>Product</th>
<th>Composition [wt%]</th>
<th>Pressure [bar G]</th>
<th>Temperature [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>para-Xylene</td>
<td>99.70 min</td>
<td>4.0</td>
<td>30</td>
</tr>
<tr>
<td>ortho-Xylene</td>
<td>99.00 min</td>
<td>4.0</td>
<td>30</td>
</tr>
</tbody>
</table>

The products are produced in *para-*xylene *ortho-*xylene ratio of 2.25 on weight basis. The by-products are a gas purge which has only a fuel value, a heavy ends stream and a light ends stream rich of benzene and toluene. The maximum allowable *ortho-*xylene content of the heavy ends stream is 20 wt%.

Additional specifications for the *para-*xylene separation units are the maximum allowable concentrations of toluene and the C₉⁺ aromatics in the feed to this separation unit. These are respectively 0.3 wt% and 0.5 wt%.

### 2.2.3 Battery limit

The battery limit of the feed and product streams and of the utilities used in this process is given in the following Table.

Table 2.4 Battery limit

<table>
<thead>
<tr>
<th>Stream</th>
<th>Temperature [°C]</th>
<th>Pressure [bar G]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed xylenes feed</td>
<td>135</td>
<td>5.0</td>
</tr>
<tr>
<td>para-Xylene product</td>
<td>30</td>
<td>4.0</td>
</tr>
<tr>
<td>ortho-Xylene product</td>
<td>30</td>
<td>4.0</td>
</tr>
<tr>
<td>C₉⁺ by-product</td>
<td>40</td>
<td>4.0</td>
</tr>
</tbody>
</table>

**Utility**

- Medium pressure steam: saturated, 12.0
- Cooling water supply: 27, 4.5
- Cooling water return: 34, 2.5
- Hydrogen make-up: ambient, *

* sufficient for compressor discharge

The L.H.V. of the fuel gas, used in the fired heater is 8870 kcal/Nm³ and the molecular weight is assumed to be 16 g/mol.

### 2.2.4 Catalyst

The catalyst used in the isomerization reactor is the Leuna Kontakt 8835. The Leuna Kontakt 8835 is
a pentasil zeolite with the MFI structure, Birke (1991). For this catalyst no kinetic data were found in literature and the Leuna Company was not willing to give this information. The activity of the catalyst can be controlled with the help of some ammonia. The bulk density of the catalyst is 630 kg/m$^3$. The particles are assumed to be spherical with a diameter of 2 mm. The lifetime of the catalyst is 3 years.

2.2.5 Reactions

The main reactions in the process are the isomerization reactions. In literature two different mechanisms were found. According to Bhatia (1989), no direct isomerization of ortho-xylene to para-xylene takes place:

$$\text{ortho-xylene} \neq \text{meta-xylene} \neq \text{para-xylene}$$ (1)

In this case isomerization of ortho-xylene to para-xylene only occurs via meta-xylene. Li (1992) assumes a mechanism where direct isomerization of all three isomers takes place:

$$\text{meta-xylene} \neq \text{ortho-xylene} = \text{para-xylene}$$ (2)

Since no kinetic data were available it is not important which mechanism should be used. Side-reactions which are reported by Bhatia (1989) and Li (1992) are hydrogenation and disproportionation of xylene. A part of the xylenes is disproportionated into toluene, benzene and C9 aromatics. Assumed is that the only C9$^+$ chemicals which are formed are trimethylbenzene, cumene and diethylbenzene. This results in the following reactions:

$$\text{2 xylene} \rightarrow \text{toluene} + \text{trimethylbenzene}$$ (3a)
$$\text{2 xylene} \rightarrow \text{toluene} + \text{cumene}$$ (3b)
$$\text{2 xylene} \rightarrow \text{benzene} + \text{diethylbenzene}$$ (3c)

It is assumed that trimethylbenzene, cumene and diethylbenzene are formed on equal mass basis.

The hydrogenation of part of the xylenes results in the formation of toluene and methane:

$$\text{xylene} + \text{H}_2 \rightarrow \text{toluene} + \text{methane}$$ (4)

It is assumed no hydrogenation of xylenes to benzene takes place. Bhatia (1989) and Li (1992) do also not report the occurrence of hydrogenation of the aromatics to cyclo-alkanes and alkanes. Since the ethylbenzene in the feed is not separated from the xylenes it is necessary to convert the ethylbenzene, to prevent a build up of ethylbenzene in the recycle. There are two possible ways to convert the ethylbenzene. Dealkylation to benzene and ethane and isomerization to xylenes. Side reactions are the disproportionation reactions into toluene or benzene and C$^+$ aromatics. The Leuna Kontakt 8835 catalys especially converts the ethylbenzene by dealkylation.
ethylbenzene + H₂ --> benzene + ethane  \hspace{1cm} (5)

The disproportionation reactions are:

\begin{align*}
2 \text{ethylbenzene} &\rightarrow \text{toluene} + \text{trimethylbenzene} \hspace{1cm} (6a) \\
2 \text{ethylbenzene} &\rightarrow \text{cumene} \hspace{1cm} (6b) \\
2 \text{ethylbenzene} &\rightarrow \text{benzene} + \text{diethylbenzene} \hspace{1cm} (6c)
\end{align*}

Because no kinetic data were obtained for the isomerization process with the Leuna Kontakt 8835 catalyst it was assumed that for the reactor conditions specified in Table 2.5 the \textit{para}-xylene approach is 0.995, the \textit{ortho}-xylene approach is 0.99 and the ethylbenzene conversion is 65 %. The equilibrium concentrations of \textit{para}-xylene and \textit{ortho}-xylene are respectively 24 wt% and 23.5 wt%, based on the total xylene amount. It is also assumed that 1% of the xylenes is hydrogenated or disproportionated and that 0.5 wt%, based on the C₆ feed to the reactor is converted into C₇⁺ aromatics. These assumptions are summarized in Table 2.5.

The approach to equilibrium can be defined as the difference between the reactor inlet and outlet concentrations divided by the difference between the equilibrium concentration and reactor inlet concentration. The concentrations for this calculation are related to the total xylene concentration. So for the \textit{para}-xylene approach the equation is:

\[
A_{PX} = \frac{(X_{PX,\text{outlet}} - X_{PX,\text{inlet}})}{(E_{PX} - X_{PX,\text{inlet}})} \hspace{1cm} 2.1
\]

where
\[
\begin{align*}
A_{PX} &\quad \text{\textit{para}-xylene approach} \\
X_{PX,\text{outlet}} &\quad \text{\textit{para}-xylene concentration at reactor outlet} \\
X_{PX,\text{inlet}} &\quad \text{\textit{para}-xylene concentration at reactor inlet} \\
E_{PX} &\quad \text{equilibrium concentration of \textit{para}-xylene}
\end{align*}
\]

Finally it is also assumed that the ratio between the conversion of \textit{para}-xylene, \textit{meta}-xylene, \textit{ortho}-xylene and ethylbenzene to trimethylbenzene, cumene and diethylbenzene is equal to the concentration ratio of \textit{para}-xylene, \textit{meta}-xylene, \textit{ortho}-xylene and ethylbenzene in the feed to the reactor.
Table 2.5 Reactor operating conditions and performance

<table>
<thead>
<tr>
<th>Reactor operating conditions</th>
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<tbody>
<tr>
<td>Inlet pressure [MPa]</td>
<td>0.85</td>
</tr>
<tr>
<td>Temperature [K]</td>
<td>668</td>
</tr>
<tr>
<td>Liquid hourly space velocity [v/vh]</td>
<td>2.5</td>
</tr>
<tr>
<td>H₂/C₆ molar ratio [mol/mol]</td>
<td>3.0</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Reactor performance</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><em>para</em>-Xylene approach</td>
<td>0.995</td>
</tr>
<tr>
<td><em>ortho</em>-Xylene approach</td>
<td>0.99</td>
</tr>
<tr>
<td>Ethylbenzene conversion</td>
<td>0.65</td>
</tr>
<tr>
<td><em>para</em>-Xylene equilibrium concentration [wt%]</td>
<td>24</td>
</tr>
<tr>
<td><em>ortho</em>-Xylene equilibrium concentration [wt%]</td>
<td>23.5</td>
</tr>
<tr>
<td>Xylene loss over reactor [wt%]</td>
<td>1.0</td>
</tr>
<tr>
<td>C₇⁺ formation [wt% based on C₆ feed]</td>
<td>0.5</td>
</tr>
</tbody>
</table>

2.3 Location of the plant

The plant is to be located at an aromatics complex in Europoort, The Netherlands
3 Process structure

The process can be divided in three sections. The first section is the separation section upstream the reaction section. In this section the products, para-xylene and ortho-xylene, are separated from the stream which is fed to the reactor. In the reaction section the mixed xylenes are isomerized to near equilibrium composition. The ethylbenzene is mainly converted to benzene and ethane. In the separation section downstream the reaction section first the hydrogen and the lowest boiling components are separated and recycled to the reaction section. Then the liquid flow is separated in a light ends stream, which is a byproduct, and a xylenes stream. This stream is recycled to the separation section upstream the reaction section. The process flow scheme of the process can be found in Appendix B. The mass and heat balances can be found in Appendix C and the stream compositions can be found in Appendix D.

The process was simulated with ChemCad III. The thermodynamic model used is the Soave-Redlich-Kwong model. This model was selected because all the components, except hydrogen, are hydrocarbons, and the process operates under moderate pressure and temperature, see De Loos (1994).

3.1 Feed streams

The feed streams of the process are:

- mixed xylenes feed
- hydrogen feed

The mixed xylenes feed originates from a refinery. This stream is delivered at 5.0 bar G and 135°C. The composition of this stream is given in Table 2.1.

The hydrogen originates from a platformer. This stream is delivered at ambient temperature, and at a pressure which is sufficient for compressor discharge. The composition of this stream is given in Table 2.2.

3.2 Separation section upstream the reactor

It is possible to separate the ethylbenzene in the feed from the xylenes by distillation. Because of the small difference in boiling point between ethylbenzene and para-xylene about 300 theoretical trays will be necessary. In this process ethylbenzene is mainly removed by conversion to benzene and ethane in the reactor, so no ethylbenzene distillation column is needed. It depends upon the market situation whether the process produces only para-xylene, or also ortho-xylene. In this process both ortho-xylene and para-xylene are produced, so a xylene splitter is necessary which splits part of the ortho-xylene from the other xylenes. A para-xylene separation unit is also present upstream the reactor to produce highly purified para-xylene.
3.2.1  *ortho*-Xylene separation and purification

The feed stream pressure is reduced with a valve to the operation pressure of the xylene splitter, T1. This stream is then mixed with the recycle stream and then fed to the xylene splitter, T1. The bottom stream of the xylene splitter are the heavy ends and part of the *ortho*-xylene. The top stream is condensed by aircooler H2. This stream consists of all the lower boiling compounds and the remaining *ortho*-xylene. The condensed stream is fed to the reflux drum V4, which has a residence time of 10 minutes, to compensate for flow changes. Pump P5 pumps part of this stream to the para-xylene separator, whereas the rest is refluxed.

The amount of *ortho*-xylene in the bottom stream defines the product ratio of *para*-xylene and *ortho*-xylene, which is set at 2.25.

The bottom stream is fed to a second distillation column, T16, where the *ortho*-xylene is purified. The top product of this column is condensed by aircooler H17. This stream is *ortho*-xylene with a purity of 99.0 wt%. Heat exchanger H24 and pump P26 bring this by-product to the specified temperature and pressure.

The bottom stream of the *ortho*-xylene column consists mainly of heavy ends. The *ortho*-xylene amount in this stream is 14.7 wt%. Heat exchanger H25 and pump P27 bring this product to the specified temperature and pressure.

3.2.2  *para*-Xylene separation

In the *para*-xylene separation unit, V8, the *para*-xylene is separated from the other compounds. Two kinds of *para*-xylene separation processes are commercially available; crystallization and adsorption. Because of the large difference in melting temperature between *para*-xylene and the other xylenes it is possible to separate the *para*-xylene with a crystallization process. A number of different crystallization processes are commercially used. These are given by Kirk Othmer (1984).

The purity of the *para*-xylene originating from the crystallization process is high, 99.7 wt%. Because of a eutectic point the maximum *para*-xylene recovery is 65%, so the filtrate of the crystallization process contains about 10 wt% *para*-xylene.

Since 1970 adsorption processes are also available for the *para*-xylene separation. The two processes that are nowadays available are PAREX, described by Thornton (1970) and ELUXYL, described by Ash (1994). The advantage of the adsorption processes compared to the crystallization processes is the high *para*-xylene recovery; the *para*-xylene concentration in the filtrate is about 1.5 wt%. The disadvantage is that the purity of the *para*-xylene originating from the adsorption process is less than the purity of a crystallization process.

A combination of these two processes can be used to have the advantage of crystallization, a high purity, as well as the advantage of adsorption, a high *para*-xylene recovery. Figure 3.1 shows the configuration for this combination, Ash (1994).

![Figure 3.1 Combination of adsorption and crystallization](image-url)
In our design two situations were examined. At first the para-xylene separation process is a crystallization process. Secondly the para-xylene separation process is the described combination of crystallization and adsorption.

In both situations the separation process was handled as a black box.

### 3.3 Reaction section

The filtrate of the para-xylene separation is fed to the reaction section. First the filtrate is pumped to the desired pressure for the reactor, by pump P11. Then the filtrate is mixed with the gas recycle. Before the stream enters the reactor it is heated with the reactor effluent in heat exchanger H15 and in fired heater F20.

The reactor, R23, used is an adiabatic fixed bed reactor. Several catalysts can be used for this reactor. The main difference between the catalysts is the way ethylbenzene is treated. The Octafining catalyst, described by Uhlig (1969), the Leuna Kontakt 8831, described by Birke (1992) and the UOP 1-200, described by Chem Systems (1992) isomerize the ethylbenzene to xylene. On the other hand some other, newer, catalysts dealkylate the ethylbenzene to benzene and ethane. Examples are the UOP 1-100, described in Chem Systems (1992) and the Leuna Kontakt 8835, described by Birke (1992).

An ethylbenzene isomerization catalyst uses an equilibrium-limited reaction to convert the ethylbenzene whereas an ethylbenzene dealkylation reaction is not equilibrium limited. For a ethylbenzene dealkylation catalyst a higher ethylbenzene conversion per pass through the xylene isomerization reactor is reached. Because of these differences the para-xylene production is higher when a dealkylation catalyst is used, although the para-xylene yield is lower. This is described by Jeanneret (1994).

The catalyst used in the reactor is the Leuna Kontakt 8835, an ethylbenzene dealkylation catalyst. The operating conditions in this process can be found in Chapter 2.

The reactor effluent is cooled with the reactor feed in H15 and with cooling water in H28 to a temperature of 49°C and led to the separation section downstream the reactor.

### 3.4 Separation section downstream the reaction section

The first unit in the separation section downstream the reaction section is the gas/liquid separator V29. The separator operates at a temperature of 49°C. This temperature was chosen to reach an optimum between the amount of xylene in the gas recycle and thus in the purge and the amount of light ends in the liquid flow.

The top stream of the gas liquid separator is recycled. A compressor, C19, compensates for the pressure drop over the reaction section. A purge is installed to prevent the build up of methane, ethane and propane. Fresh hydrogen is added to the gas recycle to maintain the desired H2/C8 ratio in the reactor.

The purge percentage should be low considering the high hydrogen prices. The purge only has a fuel value.

The bottom stream of the gas liquid separator is fed to distillation column T7. Here benzene, toluene and the light ends still present in the liquid are separated from the xylenes, ethylbenzene and the heavy ends. The column is equipped with an aircooler as partial condenser, H9. The partly condensed steam from the aircooler is fed to the gas/liquid separator, V12. The gas stream originating from this separator is the C7-product. The liquid stream is recycled to the column.

The bottom stream of this column is pumped by pump P10 to the clay tower, T14.
In the clay tower, traces of organic substances which are formed in the process and which could cause optical disturbances in the downstream products of para-xylene are removed. The stream originating from the clay tower is recycled and mixed with the feed stream of the process.
4 Equipment selection and design

4.1 Reactor

Unfortunately no kinetic data were found in literature about the performance of the catalyst used. The para-xylene and ortho-xylene approach, the ethylbenzene conversion and the reactor temperature and pressure used were provided by Raytheon Engineers and Constructors. The reactor chosen is an adiabatic, fixed bed reactor. In Appendix EI the design procedure for the reactor is given. The results can be found in Appendix K. Table 4.1 gives the most important results.

<table>
<thead>
<tr>
<th>( V_{\text{reactor}} ) [m³]</th>
<th>58.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D_{\text{reactor}} ) [mm]</td>
<td>3,500</td>
</tr>
<tr>
<td>pressure drop [mbar]</td>
<td>490</td>
</tr>
<tr>
<td>( \Delta T ) [°C]</td>
<td>4.0</td>
</tr>
</tbody>
</table>

4.2 Distillation columns

The distillation columns were simulated with ChemCadIII. A selection of the column internals had to be made. For all distillation columns structured packings were selected. The main advantages of structured packings are the dimensions of the column and a lower pressure drop. The main disadvantages of structured packings are their sensitivity to fouling and liquid maldistribution. For all columns the same packing was selected: the Sulzer Mellapak 250X. This packing has a specific area of 250 m²/m³. A packing with a higher specific area would result in a column with smaller dimensions, but will be more sensitive to fouling and more difficult to clean. A liquid redistributor was installed after each 15 theoretical stages in order to maintain a good liquid distribution, Olujic (1994).

The dimensions of the columns were calculated with the computer program SULPAK-PC 4.1 from the Sulzer company.

The design method and a example calculation can be found in Appendix EII. The results of the calculations can be found in Appendix K. Table 4.2 summarizes the most important results.
Table 4.2 Results of the distillation columns design

<table>
<thead>
<tr>
<th></th>
<th>Column T1</th>
<th>Column T7</th>
<th>Column T16</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reflux ratio</td>
<td>2.13</td>
<td>6.65</td>
<td>5.16</td>
</tr>
<tr>
<td>Number of</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>theoretical stages</td>
<td>73</td>
<td>50</td>
<td>77</td>
</tr>
<tr>
<td>Diameter top [mm]</td>
<td>3,440</td>
<td>1,340</td>
<td>1,290</td>
</tr>
<tr>
<td>Diameter bottom [mm]</td>
<td>3,440</td>
<td>1,960</td>
<td>1,290</td>
</tr>
<tr>
<td>Height [mm]</td>
<td>52,500</td>
<td>37,000</td>
<td>54,500</td>
</tr>
<tr>
<td>Pressure drop [mbar]</td>
<td>152</td>
<td>107</td>
<td>158</td>
</tr>
</tbody>
</table>

4.3 Aircoolers

In general, air is economically the best cooling medium when the temperature of the process fluid to be cooled is over 65°C, see Sinnott (1993). Since the top streams of all the columns are over 65°C, for all column condensers aircoolers were chosen. The aircoolers were designed according to Brown (1978). In Appendix EIII the general design procedure and an example calculation can be found. The effective transfer coefficient for the air film on the outside of the tube is low, indicating that some sort of fin is required, but the actual fin design is left open. Only a bare tube surface was calculated. The results of the design can be found in Appendix K. Table 4.3 gives the most important results.

Table 4.3 Results of aircooler design

<table>
<thead>
<tr>
<th></th>
<th>H2</th>
<th>H9</th>
<th>H17</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat duty [Gcal/h]</td>
<td>14.7</td>
<td>2.1</td>
<td>2.1</td>
</tr>
<tr>
<td>Mass flow [ton/h]</td>
<td>175.3</td>
<td>22.9</td>
<td>24.9</td>
</tr>
<tr>
<td>Pressure drop [mbar]</td>
<td>47</td>
<td>18</td>
<td>25</td>
</tr>
<tr>
<td>Bare tube surface [m²]</td>
<td>718.5</td>
<td>318.3</td>
<td>140.0</td>
</tr>
<tr>
<td>Fan power [kW]</td>
<td>88.2</td>
<td>39.1</td>
<td>12.8</td>
</tr>
</tbody>
</table>

4.4 Heat exchangers

For all heat exchangers and reboilers, with the exception of the aircoolers, shell and tube exchangers were used. This type of heat exchangers can be used for all applications. Because of the high temperature differences internal floating head exchangers were used. The basic design procedure and theory for this type of exchangers is presented in Appendix EIV, see Sinnott (1993). The results are presented in Appendix K. The most important results are presented in Table 4.4.
In the integrated heat exchanger upstream the reactor, H15, the reactor feed is heated by the reactor effluent. The reactor feed was totally vaporized in this heat exchanger. To calculate the effective heat transfer coefficient Chen's method was used, Sinnott (1993). The temperature difference between the two outlet streams was 10 K.

The reactor effluent leaving this integrated heat exchanger was fed to another heat exchanger, H28, where it was partly condensed. This condensor cannot be an aircooler, because the reactor effluent has to be cooled to a temperature of 49°C. In this case a water-cooled heat exchanger was used. This condenser was designed with the method of Kern, Sinnott (1993). For this condenser an example calculation was made, see Appendix EIV.

For the heat exchangers, H24 and H25, cooling water was used.

For the reboilers medium pressure steam was used. Fixed tube sheet thermosyphon reboilers were used. This type of reboiler is the most economical type for most applications. Because of the difference in density between the two-phase mixture of vapour and liquid in the heat exchanger and the single-phase liquid in the base of the column, natural circulation through the heat exchanger is maintained. Horizontal thermosyphon reboilers were used. In horizontal thermosyphon reboilers the steam flows through the tubes. In this case the shell wall does not have to resist to steam pressure. Horizontal reboilers are also easier to clean than vertical reboilers. The design method for the reboilers was obtained from Sinnott (1993). The results are presented in Appendix K. The most important results are presented in Table 4.5.

### Table 4.5 Results of reboiler design

<table>
<thead>
<tr>
<th></th>
<th>H 3</th>
<th>H 6</th>
<th>H 18</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat duty [Gcal/h]</td>
<td>14.6</td>
<td>4.3</td>
<td>2.1</td>
</tr>
<tr>
<td>Area [m²]</td>
<td>404.8</td>
<td>95.1</td>
<td>115.8</td>
</tr>
<tr>
<td>Steam flow [ton/h]</td>
<td>47.8</td>
<td>13.9</td>
<td>7.1</td>
</tr>
</tbody>
</table>
4.5 Fired heater

A choice had to be made about the type of fired heater used. A vertical-cylindrical fired heater with crossflow convection section was chosen based on the discussion of several types of fired heaters by Berman (1978a). This type of fired heater has a high economical efficiency and requires a minimum of plot area. The design of fired heater F20 was based on the design method by Berman (1978b). The design method and the calculation are given in Appendix EVI. The results are given in Appendix K. In Table 4.6, the results are summarized.

Table 4.6 Results of the fired heater design

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>capacity</td>
<td>[Gcal/h]</td>
<td>9.3</td>
</tr>
<tr>
<td>fuel consumed</td>
<td>[kg/h]</td>
<td>772</td>
</tr>
<tr>
<td>pressure drop</td>
<td>[mbar]</td>
<td>500</td>
</tr>
</tbody>
</table>

4.6 Gas/Liquid separators

The gas/liquid separators, V12 and V29, were designed according to the method described by Olujic (1994). In Appendix EVI this method can be found, as well as an example calculation. The results can be found in Appendix K. Table 4.7 gives the most important results.

4.7 Reflux drum

The reflux drums for the distillation columns T1 and T16 were designed according to the method described by Mehra (1979) and Younger (1955). In Appendix EVII this method can be found, as well as an example calculation. The results can be found in Appendix K. These are summarized in Table 4.7.

Table 4.7 Results of the gas/liquid separators and reflux drums design

<table>
<thead>
<tr>
<th></th>
<th>V4</th>
<th>V12</th>
<th>V21</th>
<th>V29</th>
</tr>
</thead>
<tbody>
<tr>
<td>type</td>
<td>reflux drum</td>
<td>gas/liquid separator</td>
<td>reflux drum</td>
<td>gas/liquid separator</td>
</tr>
<tr>
<td>position</td>
<td>horizontal</td>
<td>horizontal</td>
<td>horizontal</td>
<td>vertical</td>
</tr>
<tr>
<td>pressure [bar G]</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>6.9</td>
</tr>
<tr>
<td>volume [m³]</td>
<td>42.8</td>
<td>5.1</td>
<td>6.3</td>
<td>13.1</td>
</tr>
</tbody>
</table>

4.8 Claytower

No data were available in literature about clay-treatment. Based on discussions with several experienced process engineers, a pressure drop over the claytower of 0.5 bar was assumed. It was also assumed that the conditions of the bottom stream of distillation tower T6 are sufficient for the
claytower. The impurities which are removed in the claytower were present in such small amounts, that there was no influence on the mass balance. Since no data were available about the residence time in the claytower it was not possible to calculate the dimensions of the unit.

4.9 Pumps and compressors

In the process no special conditions or high heads are demanded by pumps, so all pumps are centrifugal pumps. The pump efficiencies were obtained from Figure 10.62, Sinnott (1993). The reflux pumps P5, P13 and P22 were not designed. The results of the design can be found in Appendix K.

The compressor, C19 is a centrifugal compressor. The total efficiency is assumed to be 0.75, see De Graauw (1994).
5. Process control

In order to ensure safe operation of the plant and a constant product stream and composition, a good process control system should be installed. In this part the process control system which was designed for this process will be discussed. This system was designed according to Stephanopoulos (1984).

5.1 Control of product streams

The para-xylene stream is assumed to originate from the separation unit at the specified temperature and pressure, so no control is needed for this product stream.

The composition of the ortho-xylene and the C₇+ stream is controlled in distillation column T16. The temperatures of these streams are controlled with cascade controllers. These controllers consist of a secondary flow controller in the cooling water stream, which compensates for changes in the cooling water flowrate, and a primary temperature controller in the product streams.

5.2 Control of distillation columns

Control of distillation column T1

In column T1, the liquid level in the bottom is controlled with a valve in stream 7. The temperature in the column is controlled with the steam flow through the reboiler. A cascade control configuration is used with a temperature controller and a flow controller. The temperature controller is the primary controller. The flow controller is the secondary controller and is used to compensate for changes in the steam flowrate. With this kind of control small variations in the steam flow rate will be compensated before there is an effect on the column temperature. The temperature controller is placed in the bottom of the column where the largest temperature gradient occurs.

The pressure in the top of the column is controlled with the cooling rate in the aircooler. The composition is controlled with the reflux ratio. A flow controller in the reflux stream controls the reflux ratio. When the pressure and composition of the column are fixed, the temperature is also fixed.

The liquid level in the reflux drum is controlled with a valve in stream 10.

Control of distillation column T7

The liquid level in the bottom of column T7 is controlled with a valve in stream 17. The temperature in the column is controlled with the steam flow through the reboiler. A cascade controller is used with a temperature controller and a flow controller.

The pressure in the top of the column is controlled with a pressure controller over the aircooler. The composition in the column is controlled with the reflux ratio. A flow controller controls the reflux ratio with a valve in the reflux stream. The liquid level in the gas/liquid separator is also controlled with the valve in the reflux stream. It is not possible to control two variables with one manipulated variable so a selective control system is needed to transfer control action from one controlled output to the other. Here override control is used. A high/low selector switch is installed. Under normal circumstances the valve in the reflux stream will control the reflux ratio and hence the top temperature, but when the liquid level in the gas/liquid separator is too high or too low, the control is switched to level control in the reflux drum.
Control of distillation column T16

The liquid level in the bottom of column T16 is controlled with a valve in stream 25. The temperature in the column is controlled with the steam flow through the reboiler. A cascade controller is used with a primary temperature controller and a secondary flow controller.

The pressure in the top of the column is controlled with the cooling rate in the aircooler. The reflux ratio is controlled with a flow controller, placed in the reflux stream.

The liquid level in the reflux drum is controlled with a valve in stream 28.

5.3 Control of heat exchangers

In heat exchanger H15 are no degrees of freedom in this heat exchanger, no variables can be controlled.

The temperature of the stream originating from the heat exchanger H28, stream 34, is controlled with a cascade controller. This cascade controller consists of a secondary flow controller in the cooling water stream and a primary temperature controller in stream 37.

5.4 Control of fired heater F20

The reactor feed is heated by a fired heater. The temperature of this feed stream is important since the reactor performance is influenced by the temperature. A cascade controller is installed with a flow controller in the fuel stream and a temperature controller in stream 30.

A fixed flow ratio controller is installed between the fuel stream and the air stream in order to ensure complete combustion.

When there is no fluid flow through the fired heater, the heat cannot be transferred easily so the temperature of the tubes will rise significantly. To prevent this from happening a low flow alarm is installed in stream 23.

5.5 Control of the reactor R23

The overall reaction in the reactor causes a temperature rise of a few degrees, so no temperature control in the reactor should be necessary. However the hydrogenation reactions which occur are rather exotherm. When the kinetics and selectivity of the catalyst change towards a much larger amount of hydrogenation the temperature in the reactor will rise. A temperature alarm is installed in the bottom of the reactor so this could be measured directly. The pressure is controlled with a valve in the reactor effluent stream, stream 31.

The H2/C4 ratio is controlled with a valve in stream 1. A composition controller will measure the ratio and adapt the hydrogen make-up stream when the H2/C4 ratio is too high or too low.
5.6 Control of gas/liquid separator G29

The pressure of the liquid stream of the gas/liquid separator is reduced to the inlet pressure of distillation column T7. This is controlled with a valve in stream 1. The liquid level in the gas/liquid separator is also controlled with this valve. An override control system is installed with a high/low selector switch: Under normal conditions the valve controls the pressure of the stream flowing to T7, but in case of a high liquid level, or a low liquid level in the gas/liquid separator, the control is switched to level control.

The pressure in the gas/liquid separator is controlled with a valve in the purge stream.

5.7 Control of Compressor C19

The compressor has a rotation speed, because this type of compressor is less expensive than a compressor with an adjustable rotation speed. To control the discharge pressure of the compressor, a by pass was installed with a valve. This valve is controlled by a pressure controller in the compressor discharge stream.
6. Process safety

6.1 Hazard and operability study

A hazard and operability study, HAZOP, was performed to make a systematic, critical, examination of
the operability of the process, see Bibo (1994). The HAZOP study indicates potential hazards that may
arise from deviations from the intended design conditions. With the help of several guide words, the
causes, consequences and actions required in case of deviations from the intended operating conditions
were obtained. The results of this study are given in Appendix FI. The process control design was
partly based on the results of this HAZOP study.

6.2 Safety analysis

The safety analysis was done according to Dow’s Fire and Explosion Index Hazard Classification
Guide (1987). This index is a step-by-step objective evaluation of the fire, explosion and reactivity
potential of process equipment and its contents. The main purposes of the Dow F&E index are:

- To quantify the expected damage of potential fire and explosion incidents in realistic terms.
- To identify equipment that would be likely to contribute to the creation or escalation of an
  accident.

The Dow F&E index attempts to determine the maximum loss that can occur to a process plant or
related facility. A loss that could be experienced under the most adverse operating conditions. The
Dow F&E index was calculated with the following equation:

\[ DI = MF \cdot UHF \]  

where

- \( DI \) = Dow’s Fire and Explosion Index
- \( MF \) = material factor
- \( UHF \) = unit hazard factor

The first step was to determine the process units which would have the greatest impact on the
magnitude of a fire or explosion. In this design the hydrogen recycle will cause the greatest impact, so
the risks of this section were studied. The hydrogen recycle includes the reactor, the gas/liquid
separator and the recycle compressor.

For this section the material factor (MF) was determined. This material factor is determined by a
variable which takes the flammability of the compound considered into account, \( N_F \), and a variable
which describes the reactivity of the compound considered, \( N_R \). The material factors for all the
components present in the system are shown in Appendix FII, Table F.6.

The MF represents the hazard of the selected material at ambient temperature and pressure. If the
process unit temperature is above 333.15 K, the MF will be adjusted.

Since the flash points of all the components are below the reactor temperature, a value of 1 had to be
added to \( N_F \). When the corrected \( N_F \) was equal to 5, the value used was 4, since \( N_F \) cannot be greater
than 4. The \( N_F \)-factors and the material factors after correction are shown in Appendix FII Table F.7.

The MF of the section was taken to be that of the most hazardous substance present in the unit, so the
material factor for this section is 21.
The unit hazard factor (UHF) can be calculated with equation 6.2

\[ UHF = F_1 \cdot F_2 \]

where 

- \( F_1 \) = general process hazards factor 
- \( F_2 \) = special process hazards factor

General process hazards determine the magnitude of a loss incident. The calculation of the general process hazards factor is given in Appendix FII. The factor is 2.65.

Special process hazards determine the probability of a loss incident. The calculation of the special process hazards factor is given in Appendix FII. The factor is 3.96.

With equation 6.2 the unit hazard factor was determined to be 10.49. The unit hazard factor has a range from 1 to 8. Since the unit hazard factor obtained is larger than 8, the maximum of 8.0 is used.

From equation 6.1 it followed that the Dow's Fire and Explosion Index is 168, on a scale from 1 to 320. Because of the presence of hydrogen and hydrocarbons above their flashpoint, it is a rather dangerous process.

With this DI and Figure 8, Dow F&EI (1987) the “exposure radius” was determined. This exposure radius represents an area of exposure, the area containing equipment that could be exposed to a fire or to a fuel-air explosion generated in the process section being evaluated. Although it is known that a fire or explosion incident does not spread out in a perfect circle, the circle provides a good basis for further calculation of values. The exposure radius for this particular case was about 43 m.

The unit damage factor, UDF, was determined from the unit hazard factor, UHF, and the material factor (MF). From Figure 7, Dow F&EI (1987) it followed that the UDF = 0.83. This UDF represents the overall effect of fire plus blast damage resulting from a release of fuel or reactive energy from a process unit. This factor varies from 0.01 to 1. Here again one can say that the process considered is rather dangerous.

In the analysis as done above, no attention was given to the so called “loss control credit factors”, the value of the area of exposure, the “base maximum probable property damage (base MPPD)” and “maximum probable days outage (MPDO)”. This, because many details concerning plant layout and plant value were not available.

Overall the conclusion can be drawn that the process unit considered is rather dangerous. When looking at the different penalties which are assigned to this process unit and the factors which influence the UHF, the following remarks can be made:

**General process hazards factor:**
- The penalty taken into account for drainage and spill control is the maximum penalty possible. When attention is given to this item in the final design, this penalty can be reduced.

**Special process hazards factor:**
- The penalty taken into account for the fact that there is a possibility for air to leak into the system is the maximum penalty. Probably in the final design the probability will be reduced, because the combination of oxygen and hydrogen in one unit is very dangerous. In that case
this penalty should be reduced.

- The penalty taken into account for corrosion is an average penalty. Fact is that the substances present in the process unit are not very corrosive; for all the units carbon steel could be used as a construction material. So when it turns out that the corrosion rates are less than 0.5 mm/year, this penalty should be reduced to 0.10
- The penalty taken into account for the use of a fired heater is determined by assuming a distance from a possible leak source of 105 feet. When in the final design and plant layout the fired heater is placed further than 210 feet from a possible leak source, this penalty could be reduced to 0.10.

When these remarks are implemented in the final design the General Process Hazards Factor reduces to 2.15 and the Special Process Hazards Factor reduces to 3.06. In this case the UHF becomes 6.58. As one can see, the UDF is reduced with 0.04 points. In this case DI = 138.2, the exposure radius is 35.4 m, and the UDF = 0.79.

In conclusion it can be said that the calculated fire and explosion risks can be reduced, although it is still a rather dangerous process.
7. Economics

For the economical analysis the methods described in Montfoort (1991) were used. The following assumptions were made:

- production time: 8000 hours/year
- plant life: 10 years
- capital charge: 14.9 %
- construction time: 1 year

The results of the economical analysis are presented in this chapter. The calculations are presented in Appendix H.

7.1 Costs

The total costs consist of the production volume related costs, the operating labour related costs and the total investment costs.

The production volume related costs were 30.4 M$/year, and form the largest part of the total costs.

The operating labour related costs were 0.29 M$/year.

The total investment costs were calculated with three different methods. The results of the different methods are summarized in Table 7.1.

Table 7.1 Results of investment costs calculations

<table>
<thead>
<tr>
<th>Method</th>
<th>Total investments $I_T$ in M$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zevnik-Buchanan</td>
<td>35.66</td>
</tr>
<tr>
<td>Wilson</td>
<td>57.60</td>
</tr>
<tr>
<td>Taylor</td>
<td>42.65</td>
</tr>
<tr>
<td>Average</td>
<td>45.30</td>
</tr>
</tbody>
</table>

The method of Zevnik-Buchanan gives the lowest investment costs. However, because of the great recycle stream in the process, this method is not very reliable. The method of Wilson gives the highest investment costs. This method uses an average price for all the units, independent of complexity of an unit. The method of Taylor also includes the complexity of the process, and therefore gives a more realistic estimation of the investment costs. For the following calculations the average of these three methods will be used.

The total costs are 47.7 M$/year.

7.2 Income

The total income consist of the income from the two main products, para-xylene and ortho-xylene, and the two by-products, $C_7^+-$stream and $C_9^+$-stream.
Because of the growing demand for para-xylene and the growing production capacity the price for para-xylene is rather fluctuating. For the calculation of the total income the following prices were assumed:

- para-xylene 500 $/ton
- ortho-xylene 400 $/ton
- C_7-Stream 150 $/ton
- C_9*-Stream 200 $/ton

The total income is 52.5 M$/year.

The annual profit before taxes is the total income minus the total costs.

The annual profit is 4.8 M$.

7.3 Economical criteria

To determine the process profitability, several criteria can be used. The following three criteria were determined: the Return On Investment, ROI, the Internal Rate of Return, IRR and the Pay-Out-Time, POT.

The ROI gives the percentage of the investments which is returned annually, the IRR gives the percentage of investments which is returned annually, taking into account the change in value of money over the years, and the POT is the time required to recover the fixed capital investments.

For a plant life of 10 years the ROI and the IRR should at least be 10%. An acceptable POT is 18 - 24 months, Montfoort (1991). The calculated criteria are given in Table 7.2.

<table>
<thead>
<tr>
<th>Table 7.2 Economical criteria</th>
</tr>
</thead>
<tbody>
<tr>
<td>ROI</td>
</tr>
<tr>
<td>IRR</td>
</tr>
<tr>
<td>POT</td>
</tr>
</tbody>
</table>

Based on these economical criteria it can be concluded that the process is profitable.
Effects of an additional adsorption unit

When the para-xylene isomerization plant design was completed, the effects of an additional adsorption unit on the plant were determined. The adsorption unit increased the para-xylene recovery in the para-xylene separation unit from 65 % to 95 %, so the para-xylene concentration in the filtrate will decrease from 10 wt% to about 1.5 wt%. The feed to the plant was increased to 20,500 kg/h, an increase of 26 %. This increase ensured that the volumetric flow to the reactor in the new situation deviated less than 1 % of the volumetric flow in the original design. The new mass and energy balance can be found in Appendix CII. The stream compositions can be found in Appendix DII. Appendix L gives an overview of the heat duties, the pump and compressor powers and the diameters of the distillation columns for the old as well as the new situation.

It was assumed that the reactor has the same LHSV in the new situation as in the old situation. Since no kinetic data were available, it was assumed that the reactor performance resulted in the same approaches and conversions.

An overview of the different feed and product streams is given in Table 8.1.

<table>
<thead>
<tr>
<th>Stream</th>
<th>Flow in situation 1 [kg/h]</th>
<th>Flow in situation 2 [kg/h]</th>
<th>Relative increase [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed xylenes feed</td>
<td>16,250</td>
<td>20,500</td>
<td>26</td>
</tr>
<tr>
<td>Hydrogen feed</td>
<td>904</td>
<td>914</td>
<td>1</td>
</tr>
<tr>
<td>para-Xylene product</td>
<td>8,893</td>
<td>12,680</td>
<td>43</td>
</tr>
<tr>
<td>ortho-Xylene product</td>
<td>4,044</td>
<td>3,844</td>
<td>-5</td>
</tr>
<tr>
<td>Heavy ends</td>
<td>275</td>
<td>252</td>
<td>-8</td>
</tr>
<tr>
<td>Light ends</td>
<td>2978</td>
<td>3538</td>
<td>19</td>
</tr>
<tr>
<td>Purge</td>
<td>968</td>
<td>1115</td>
<td>15</td>
</tr>
</tbody>
</table>

As can be seen from Table 8.1, an increase of 26 % of the feed resulted in an increase of 43 % of the para-xylene production. The ortho-xylene production decreased with 200 kg/h, 5 %. When the ortho-xylene production in the new situation equals the old situation the para-xylene flow will be 200 kg/h lower and the para-xylene production capacity will increase with 40 %.

As can be seen in Appendix L, all units can be used in the new situation. The heat duties of the heat exchangers and the air coolers are all less in the new situation. The capacities of the existing pumps and compressor are sufficient for the new situation. The calculated diameters of the distillation columns are between 3 % and 5 % smaller in the new situation. So the gas and liquid velocities in the columns will be lower in situation 2. Since the difference in column diameter is maximum 5 %, there will be no weeping danger.

The only specification that cannot be met is the toluene concentration in the stream flowing to the para-xylene separation unit. The toluene concentration in the mixed xylenes feed is 1 wt%. The maximum allowable toluene concentration in the feed to the para-xylene separation unit is 0.3 wt%. In the old situation, recycle stream 5 was 2.7 times the mixed xylenes feed. Since the toluene amount in
stream 5 was small, the toluene concentration in stream 4 is diluted to 0.3 wt%. No toluene is present in the bottom stream of T1, so the toluene concentration in the feed to the para-xylene separation unit is 0.3 wt%.

In the new situation, recycle stream 5 is only 1.9 times the mixed xylenes feed, so the toluene concentration in the feed to the para-xylene separation unit becomes 0.4 wt%. It is not possible to reach the limit of 0.3 wt% toluene in the feed to the para-xylene separation unit if the mixed xylenes feed is increased and the recycle stream is maintained.

The only possibility to get a toluene concentration of 0.3 wt% is to remove part of the toluene from the mixed xylenes feed before it enters the process.

It is not possible to increase the para-xylene production capacity more than calculated with the same units. As can be seen in Table L.1 the heat duties of air cooler H2 and reboiler H3 in the new situation deviated less than 1% from the heat duties in the old situation. When the feed is increased more the heat duties of these units will be insufficient.

The para-xylene production capacity could be more increased when the capacity of these two units is increased, as will be stated below.

The volumetric flow to the reactor in the new situation maintained, but the composition is different. The increase of the mixed xylenes feed results in a higher amount of xylenes and ethylbenzene in the feed to the para-xylene separation unit. Since the adsorption unit has a higher para-xylene recovery percentage than the crystallization unit, the total amount of xylenes after the para-xylene separation unit in the new situation is almost equal to the old situation.

The adsorption unit does not decrease the amount of ethylbenzene, so the ethylbenzene concentration in stream 15 is increased. This increase is 27%.

Part of the ethylbenzene is converted to benzene and ethane in the reactor. In this reaction hydrogen is consumed. When the amount of ethylbenzene is increased, the hydrogen consumed is also increased, so more fresh hydrogen is needed. Since the hydrogen feed contains 20 vol% light hydrocarbons, the amount of light hydrocarbons in the feed to the reactor is also increased. These components do not react, so the gas recycle increases. Since the total volumetric flow to the reactor does not change, the xylene concentration decreases. As a result of this the liquid flow from the gas/liquid separator V29 decreases.

The larger gas recycle causes the required power for compressor C19 to increase with 0.7%.

When the gas purge percentage is increased, the gasrecycle will decrease, so the xylene concentration can be raised by a few percent, and hence the feed can be raised. This results in a larger flow downstream the reactor.

As can be seen in Appendix L, the capacity of all the units except H2 and H3, in the new situation, are sufficient for an even larger flow. An increase of the capacity of H2 and H3 is necessary to raise the para-xylene production capacity.
9. Conclusions and recommendations

A short term and a long term strategy were examined to increase the para-xylene production for a grassroots aromatics complex. The main products were para-xylene and ortho-xylene which were produced with a minimum purity of respectively 99.70 wt% and 99.00 wt%.

The short term strategy was to use a new catalyst, the Leuna Kontakt 8835. For a fresh mixed xylenes feed of 130,000 ton/year this resulted in a para-xylene production of 71,140 ton/year and an ortho-xylene production of 32,350 ton/year.

The long term strategy was to add an adsorption unit to the existing para-xylene crystallization unit. This resulted in an increase of 26 % of fresh mixed xylenes feed to 164,000 ton/year. In this situation the production of para-xylene increased with 43 % to 101,440 ton/year and the ortho-xylene production became 30,750 ton/year.

Although the capacity of the plant is increased, the capacities and heat duties of all units are still sufficient. The heat duties of aircooler H2 and reboiler H3 will become insufficient when the para-xylene production is further increased. Because of a higher amount of ethylbenzene in the feed to the reactor the gas-recycle will be larger. Since the volumetric flow to the reactor is maintained, this results in a lower liquid flow from the gas/liquid separator V29.

The specification of maximum 0.3 wt% toluene in the feed to the para-xylene separation unit cannot be met when the mixed xylenes feed is increased. In order to meet this specification, part of the toluene should be removed from the mixed xylenes feed before it enters the process.

For the design without the adsorption unit an economical analysis was made. A para-xylene price of 500 $/ton was assumed. This resulted in an annual profit of $ 4,800,000. The Return On Investment and the Internal Rate of Return were respectively 12.4 % and 13 %. The Pay-Out-Time was 20 months.

The results of this study on the effects of an additional adsorption unit show a large increase in the para-xylene production with almost no bottle necks occurring in the process. It is therefore recommended to make a more detailed study. An economical analysis has to be made as well.

A rather large amount of expensive hydrogen is purged. It could be examined whether a hydrogen separation unit, for example an oil wash, would be profitable.
10. Literature


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11. Nomenclature

Appendix EI : Design of the reactor

\[ \Delta p \] Pressure drop \[ \text{[Pa]} \]
\[ \varepsilon \] Porosity \[ \text{[-]} \]
\[ \mu \] Viscosity \[ \text{[Pa.s]} \]
\[ p_g \] Gas density \[ \text{[kg/m}^3\text{]} \]
\[ \phi_{V,60^\circ F} \] Liquefied volume stream to the reactor at 60°F \[ \text{[m}^3\text{/h]} \]
\[ c_{pi} \] Heat capacity of component i \[ \text{[J/mol/K]} \]
\[ d_p \] Diameter of the particles \[ \text{[m]} \]
\[ h \] Height of the reactor \[ \text{[m]} \]
\[ H_{298K} \] Enthalpy of formation of component i at 298K \[ \text{[J/mol]} \]
\[ LHSV \] Liquid Hourly Space Velocity \[ \text{[h]} \]
\[ n \] Number of components \[ \text{[-]} \]
\[ T_e \] Temperature at the reactor entrance \[ \text{[K]} \]
\[ T_o \] Temperature at the reactor outlet \[ \text{[K]} \]
\[ v \] Superficial velocity \[ \text{[m/s]} \]
\[ V_{reactor} \] Volume of the reactor \[ \text{[m}^3\text{]} \]
\[ x_{i,o} \] Mole fraction of component i at the reactor outlet \[ \text{[-]} \]
\[ x_{i,e} \] Mole fraction of component i at the reactor inlet \[ \text{[-]} \]

Appendix EII : Design of the distillation columns

\[ D_{col} \] Column diameter \[ \text{[m]} \]
\[ h_{col} \] Total column height \[ \text{[m]} \]
\[ h_{pb} \] Height of the packed bed \[ \text{[m]} \]
\[ h_{red} \] Total height required for the redistributors \[ \text{[m]} \]
\[ h_a \] Height required to remove top and bottom streams \[ \text{[m]} \]

Appendix EIII : Design of the aircoolers

\[ \Delta P \] Pressure drop for total gas flow \[ \text{[psi]} \]
\[ \Delta t_1 \] Least temperature difference at inlet or outlet \[ \text{[°F]} \]
\[ \Delta t_2 \] Greatest temperature difference at inlet or outlet \[ \text{[°F]} \]
\[ \Delta T_{lm,corr} \] Corrected log mean temperature difference \[ \text{[°F]} \]
\[ \Delta T_{lm} \] Log mean temperature difference \[ \text{[°F]} \]
\[ \rho_{gas} \] Fluid gas density \[ \text{[lb/ft}^3\text{]} \]
\[ \varphi_{mf} \] Fluid mass flow \[ \text{[lb/s]} \]
\[ A \] Hypothetical bare-tube surface \[ \text{[ft}^2\text{]} \]
\[ A \] Total bare tube surface \[ \text{[ft}^2\text{]} \]
\[ A_{cross} \] Total cross section of the tubes \[ \text{[ft}^2\text{]} \]
\[ A_{tube} \] Surface of one tube \[ \text{[ft}^2\text{]} \]
\[ c_{TVD} \] Mean temperature difference correction factor \[ \text{[-]} \]
\[ D_i \] Tube inner diameter \[ \text{[ft]} \]
\[ f_f \] Friction factor \[ \text{[-]} \]
### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L_{\text{hydr}}$</td>
<td>Hydraulic length</td>
<td>[ft]</td>
</tr>
<tr>
<td>$n_{\text{total}}$</td>
<td>Total number of tubes</td>
<td>[-]</td>
</tr>
<tr>
<td>$P$</td>
<td>Temperature efficiency</td>
<td>[-]</td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat duty</td>
<td>[Btu/h]</td>
</tr>
<tr>
<td>$R$</td>
<td>Correlating factor</td>
<td>[-]</td>
</tr>
<tr>
<td>$t_1$</td>
<td>Inlet air temperature</td>
<td>[°F]</td>
</tr>
<tr>
<td>$t_2$</td>
<td>Outlet air temperature</td>
<td>[°F]</td>
</tr>
<tr>
<td>$T_1$</td>
<td>Outlet fluid temperature</td>
<td>[°F]</td>
</tr>
<tr>
<td>$T_2$</td>
<td>Inlet fluid temperature</td>
<td>[°F]</td>
</tr>
<tr>
<td>$U$</td>
<td>Overall heat transfer coefficient</td>
<td>[Btu/h/ft²/°F]</td>
</tr>
<tr>
<td>$v_{\text{gas}}$</td>
<td>Fluid gas velocity</td>
<td>[ft/s]</td>
</tr>
</tbody>
</table>

### Appendix EIV: Design of the heat exchangers

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Gamma_h$</td>
<td>Tube loading</td>
<td>[kg/m/s]</td>
</tr>
<tr>
<td>$\Delta P_s$</td>
<td>Pressure drop on the shell-side</td>
<td>[N/m²]</td>
</tr>
<tr>
<td>$\Delta P_t$</td>
<td>Tube-side pressure drop</td>
<td>[N/m²]</td>
</tr>
<tr>
<td>$\Delta T$</td>
<td>Allowed heat-up of the cooling water</td>
<td>[°C]</td>
</tr>
<tr>
<td>$\Delta T_{lm}$</td>
<td>Log mean temperature difference</td>
<td>[°C]</td>
</tr>
<tr>
<td>$\Delta T_m$</td>
<td>Mean temperature difference</td>
<td>[°C]</td>
</tr>
<tr>
<td>$\mu_l$</td>
<td>Liquid viscosity</td>
<td>[N·s/m²]</td>
</tr>
<tr>
<td>$\mu_v$</td>
<td>Vapour viscosity</td>
<td>[N·s/m²]</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density of fluid</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>$\rho_l$</td>
<td>Liquid density</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>Vapour density</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>$1/X_{\mu}$</td>
<td>Lockhart-Martelli two-phase flow parameter</td>
<td>[-]</td>
</tr>
<tr>
<td>$A$</td>
<td>Heat-transfer area</td>
<td>[m²]</td>
</tr>
<tr>
<td>$A_c$</td>
<td>Cross-flow area</td>
<td>[m²]</td>
</tr>
<tr>
<td>$A_t$</td>
<td>Area of one tube</td>
<td>[m²]</td>
</tr>
<tr>
<td>$c_{\text{water}}$</td>
<td>Heat capacity of water</td>
<td>[kJ/kg/°C]</td>
</tr>
<tr>
<td>$d_e$</td>
<td>Equivalent diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$d_i$</td>
<td>Tube inner diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$d_o$</td>
<td>Tube outer diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$D_b$</td>
<td>Bundle diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$D_p$</td>
<td>Outlet pipe diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$D_s$</td>
<td>Shell diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>$f_e$</td>
<td>Factor to account for the effects of two-phase flow</td>
<td>[-]</td>
</tr>
<tr>
<td>$f_s$</td>
<td>Suppression factor (accounts for the fact that nucleate boiling is more difficult in a flowing liquid)</td>
<td>[-]</td>
</tr>
<tr>
<td>$F_t$</td>
<td>Temperature correction factor</td>
<td>[-]</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
<td>[m/s²]</td>
</tr>
<tr>
<td>$G$</td>
<td>Total mass flow rate per unit flow area</td>
<td>[kg/m²/s]</td>
</tr>
<tr>
<td>$h_{fc}$</td>
<td>Forced convection coefficient assuming liquid fase is in conduit alone</td>
<td>[W/m²/°C]</td>
</tr>
<tr>
<td>$h_i$</td>
<td>Inside fluid film coefficient</td>
<td>[W/m²/°C]</td>
</tr>
<tr>
<td>$h_{id}$</td>
<td>Inside dirt coefficient</td>
<td>[W/m²/°C]</td>
</tr>
<tr>
<td>$h_{n_b}$</td>
<td>Nucleate boiling coefficient</td>
<td>[W/m²/°C]</td>
</tr>
<tr>
<td>$h_o$</td>
<td>Effective outside heat-transfer coefficient</td>
<td>[W/m²/°C]</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>--------</td>
<td>------------------------------------------------------------------------------</td>
<td>----------------------</td>
</tr>
<tr>
<td>$h_o$</td>
<td>Outside fluid film coefficient</td>
<td>[W/m²°C]</td>
</tr>
<tr>
<td>$h_{od}$</td>
<td>Outside dirt coefficient (fouling factor)</td>
<td>[W/m²°C]</td>
</tr>
<tr>
<td>$j_f$</td>
<td>Friction factor</td>
<td>[-]</td>
</tr>
<tr>
<td>$j_h$</td>
<td>Heat transfer factor</td>
<td>[-]</td>
</tr>
<tr>
<td>$k_f$</td>
<td>Thermal conductivity</td>
<td>[W/m°C]</td>
</tr>
<tr>
<td>$k_t$</td>
<td>Condensate thermal conductivity</td>
<td>[W/m°C]</td>
</tr>
<tr>
<td>$k_w$</td>
<td>Thermal conductivity of the tube wall material</td>
<td>[W/m°C]</td>
</tr>
<tr>
<td>$K_t$</td>
<td>Constant</td>
<td>[-]</td>
</tr>
<tr>
<td>$l_h$</td>
<td>Baffle spacing</td>
<td>[m]</td>
</tr>
<tr>
<td>$L$</td>
<td>Tube length</td>
<td>[m]</td>
</tr>
<tr>
<td>$n_t$</td>
<td>Constant</td>
<td>[-]</td>
</tr>
<tr>
<td>$N_p$</td>
<td>Number of tube-side passes</td>
<td>[-]</td>
</tr>
<tr>
<td>$N_r$</td>
<td>Average number of tubes in a vertical tube row</td>
<td>[-]</td>
</tr>
<tr>
<td>$N_t$</td>
<td>Total number of tubes in the bundle</td>
<td>[-]</td>
</tr>
<tr>
<td>$p_t$</td>
<td>Tube pitch</td>
<td>[m]</td>
</tr>
<tr>
<td>$P$</td>
<td>Operating pressure</td>
<td>[bar]</td>
</tr>
<tr>
<td>$P_c$</td>
<td>Liquid critical pressure</td>
<td>[bar]</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
<td>[-]</td>
</tr>
<tr>
<td>$q$</td>
<td>Heat flux</td>
<td>[W/m²]</td>
</tr>
<tr>
<td>$Q$</td>
<td>Heat transfer per unit time</td>
<td>[W]</td>
</tr>
<tr>
<td>$Q^*$</td>
<td>Heat flux</td>
<td>[kW/m²]</td>
</tr>
<tr>
<td>$R$</td>
<td>Dimensionless temperature ratio</td>
<td>[-]</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds number</td>
<td>[-]</td>
</tr>
<tr>
<td>$Re_l$</td>
<td>Liquid Reynolds number</td>
<td>[-]</td>
</tr>
<tr>
<td>$S$</td>
<td>Dimensionless temperature ratio</td>
<td>[-]</td>
</tr>
<tr>
<td>$t$</td>
<td>Water temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$t_i$</td>
<td>Inlet tube-side temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$t_2$</td>
<td>Outlet tube-side temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$T$</td>
<td>Mean shell-side temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$T_i$</td>
<td>Inlet shell-side temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$T_2$</td>
<td>Outlet shell-side temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$T_b$</td>
<td>Boiling temperature of liquid at bottom-pressure</td>
<td>[°C]</td>
</tr>
<tr>
<td>$T_r$</td>
<td>Reduced temperature</td>
<td>[-]</td>
</tr>
<tr>
<td>$T_{sat}$</td>
<td>Steam saturation temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$T_w$</td>
<td>Wall temperature</td>
<td>[°C]</td>
</tr>
<tr>
<td>$u_i$</td>
<td>Shell-side velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$u_t$</td>
<td>Tube-side velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>$W_c$</td>
<td>Total condensate flow</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>$x$</td>
<td>Mass fraction of vapour</td>
<td>[-]</td>
</tr>
</tbody>
</table>

Appendix EV: Design of the fired heater

- **$\Delta p$** = Pressure drop  [psi]
- **$\Delta T_{LM}$** = Log mean temperature difference  [°F]
- **$\eta$** = Efficiency  [-]
FVO 3181  Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>μ</td>
<td>Viscosity of the fluid</td>
<td>[lb/ft/hr]</td>
</tr>
<tr>
<td>ρ</td>
<td>Density of the fluid</td>
<td>[lb/ft³]</td>
</tr>
<tr>
<td>φ_m</td>
<td>Fluid mass flow</td>
<td>[lb/hr]</td>
</tr>
<tr>
<td>A</td>
<td>Heat transfer area</td>
<td>[ft²]</td>
</tr>
<tr>
<td>A_f</td>
<td>Fin surface of extended-surface tube</td>
<td>[ft²/ft]</td>
</tr>
<tr>
<td>A_b</td>
<td>Surface area of the fin bank</td>
<td>[ft²]</td>
</tr>
<tr>
<td>A_fr</td>
<td>Surface area of one finned row</td>
<td>[ft²]</td>
</tr>
<tr>
<td>A_t</td>
<td>Internal tube surface</td>
<td>[ft²/ft]</td>
</tr>
<tr>
<td>A_o</td>
<td>External tube surface</td>
<td>[ft²/ft]</td>
</tr>
<tr>
<td>A_rad</td>
<td>Radiant section surface</td>
<td>[ft²]</td>
</tr>
<tr>
<td>A_sh</td>
<td>Surface area of one shield row</td>
<td>[ft²]</td>
</tr>
<tr>
<td>A_t</td>
<td>Total surface of finned tube</td>
<td>[ft²/ft]</td>
</tr>
<tr>
<td>c_p</td>
<td>Specific heat of the fluid</td>
<td>[Btu/lb/°F]</td>
</tr>
<tr>
<td>D_i</td>
<td>Inner diameter of the tubes</td>
<td>[ft]</td>
</tr>
<tr>
<td>D_o</td>
<td>Outer tube diameter</td>
<td>[ft]</td>
</tr>
<tr>
<td>E</td>
<td>Fin efficiency</td>
<td>[-]</td>
</tr>
<tr>
<td>f</td>
<td>Fanning friction factor</td>
<td>[-]</td>
</tr>
<tr>
<td>f_r</td>
<td>Fraction radiative loss</td>
<td>[-]</td>
</tr>
<tr>
<td>G</td>
<td>Fluid mass velocity</td>
<td>[lb/hr/ft²]</td>
</tr>
<tr>
<td>G_fg</td>
<td>Flue gas mass velocity</td>
<td>[lb/hr²/°F]</td>
</tr>
<tr>
<td>h_e</td>
<td>Convection film coefficient</td>
<td>[Btu/hr²/°F]</td>
</tr>
<tr>
<td>h_i</td>
<td>In-tube film coefficient</td>
<td>[Btu/hr²/°F]</td>
</tr>
<tr>
<td>h_g</td>
<td>Gas radiation coefficient</td>
<td>[Btu/hr²/°F]</td>
</tr>
<tr>
<td>h_w</td>
<td>Tube wall coefficient</td>
<td>[Btu/hr²/°F]</td>
</tr>
<tr>
<td>H_aBWT</td>
<td>Heat available at the bridgewall temperature</td>
<td>[Btu/lb]</td>
</tr>
<tr>
<td>H_a</td>
<td>Heat available at shield bank</td>
<td>[Btu/lb]</td>
</tr>
<tr>
<td>H_fGT</td>
<td>Heat available at the flue gas temperature</td>
<td>[Btu/lb]</td>
</tr>
<tr>
<td>J</td>
<td>Heat transfer factor</td>
<td>[-]</td>
</tr>
<tr>
<td>k</td>
<td>Thermal conductivity of the flue gas</td>
<td>[ft·Btu/hr²/°F]</td>
</tr>
<tr>
<td>K_m</td>
<td>Thermal conductivity of the wall</td>
<td>[in·Btu/hr²/°F]</td>
</tr>
<tr>
<td>l_rad</td>
<td>Length of a tube in the radiant section</td>
<td>[ft]</td>
</tr>
<tr>
<td>l_sh</td>
<td>Effective length of one shield row</td>
<td>[ft]</td>
</tr>
<tr>
<td>LHV_fuel</td>
<td>Liquid heating value of the fuel</td>
<td>[Btu/lb]</td>
</tr>
<tr>
<td>L_hyd</td>
<td>Total hydraulic length of the heater</td>
<td>[ft]</td>
</tr>
<tr>
<td>n_p</td>
<td>Number of passes</td>
<td>[-]</td>
</tr>
<tr>
<td>n_r</td>
<td>Number of finned rows</td>
<td>[-]</td>
</tr>
<tr>
<td>n_t_rad</td>
<td>Number of tubes in the radiant section</td>
<td>[-]</td>
</tr>
<tr>
<td>n_t_sh</td>
<td>Number of tubes per shield row</td>
<td>[-]</td>
</tr>
<tr>
<td>q_r</td>
<td>Average radiant rate</td>
<td>[Btu/hr²]</td>
</tr>
<tr>
<td>Q</td>
<td>Transferred heat</td>
<td>[Btu/hr²]</td>
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<tr>
<td>Q_f</td>
<td>Heat absorbed by process fluid</td>
<td>[Btu/hr²]</td>
</tr>
<tr>
<td>Q_t</td>
<td>Total heat fired</td>
<td>[Btu/hr²]</td>
</tr>
<tr>
<td>Q_sh</td>
<td>Heat duty of the fin bank</td>
<td>[Btu/hr²]</td>
</tr>
<tr>
<td>Q_rad</td>
<td>Radiant section heat duty</td>
<td>[Btu/hr²]</td>
</tr>
<tr>
<td>Q_c</td>
<td>Convective heat duty of the shield bank</td>
<td>[Btu/hr²]</td>
</tr>
<tr>
<td>R_f</td>
<td>External film resistance</td>
<td>[hr·ft²·°F/Btu]</td>
</tr>
<tr>
<td>Re</td>
<td>Reynolds number</td>
<td>[-]</td>
</tr>
<tr>
<td>R_i</td>
<td>In-tube film resistance</td>
<td>[hr·ft²·°F/Btu]</td>
</tr>
<tr>
<td>R_w</td>
<td>Tube-wall resistance</td>
<td>[hr·ft²·°F/Btu]</td>
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### Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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</thead>
<tbody>
<tr>
<td>( t_w )</td>
<td>Thickness of the tube wall</td>
<td>[in]</td>
</tr>
<tr>
<td>( T_{fg} )</td>
<td>Flue gas temperature</td>
<td>[°F]</td>
</tr>
<tr>
<td>( T_{ave} )</td>
<td>Average flue gas temperature</td>
<td>[°R]</td>
</tr>
<tr>
<td>( U )</td>
<td>Overall heat transfer coefficient</td>
<td>[Btu/h/ft²/°F]</td>
</tr>
<tr>
<td>( v )</td>
<td>Fluid velocity</td>
<td>[ft/s]</td>
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**Appendix EVI: Design of a gas/liquid separator**

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<th>Symbol</th>
<th>Description</th>
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<td>( \rho_g )</td>
<td>Gas density</td>
<td>[kg/m³]</td>
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<tr>
<td>( \rho_l )</td>
<td>Liquid density</td>
<td>[kg/m³]</td>
</tr>
<tr>
<td>( C_{\text{drum}} )</td>
<td>Capacity coefficient</td>
<td>[m³/s]</td>
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<tr>
<td>( d )</td>
<td>Diameter of the separator</td>
<td>[m]</td>
</tr>
<tr>
<td>( h )</td>
<td>Height of the separator</td>
<td>[m]</td>
</tr>
<tr>
<td>( h_{fg} )</td>
<td>Height of the separator above the feed inlet</td>
<td>[m]</td>
</tr>
<tr>
<td>( h_l )</td>
<td>Height of the liquid level</td>
<td>[m]</td>
</tr>
<tr>
<td>( h_{lf} )</td>
<td>Distance between maximum liquid level and feed inlet</td>
<td>[m]</td>
</tr>
<tr>
<td>( M_g )</td>
<td>Mass flow of gas</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>( u )</td>
<td>Allowable gas velocity</td>
<td>[m/s]</td>
</tr>
<tr>
<td>( V_l )</td>
<td>Volume of liquid</td>
<td>[m³]</td>
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**Appendix EVII: Design of a reflux drum for a distillation column**

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<td>( \phi_v )</td>
<td>Volume stream out of the condensor</td>
<td>[m³/s]</td>
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<tr>
<td>( t_{\text{surge}} )</td>
<td>Surge time</td>
<td>[s]</td>
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<tr>
<td>( V_{\text{surge}} )</td>
<td>Surge volume</td>
<td>[m³]</td>
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**Appendix F: Process Safety**

<table>
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<td>( DI )</td>
<td>Dow's Fire and Explosion Index</td>
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<tr>
<td>( F_1 )</td>
<td>General process hazards factor</td>
<td>[-]</td>
</tr>
<tr>
<td>( F_2 )</td>
<td>Special process hazards factor</td>
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</tr>
<tr>
<td>( MF )</td>
<td>Material Factor</td>
<td>[-]</td>
</tr>
<tr>
<td>( MPDO )</td>
<td>Maximum Probable Days Outage</td>
<td>[-]</td>
</tr>
<tr>
<td>( MPPD )</td>
<td>Maximum Probable Property Damage</td>
<td>[-]</td>
</tr>
<tr>
<td>( N_f )</td>
<td>Degree of flammability</td>
<td>[-]</td>
</tr>
<tr>
<td>( N_R )</td>
<td>Degree of reactivity</td>
<td>[-]</td>
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<tr>
<td>( UDF )</td>
<td>Unit Damage Factor</td>
<td>[-]</td>
</tr>
<tr>
<td>( UHF )</td>
<td>Unit Hazard Factor</td>
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**Appendix H: Economics**

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<td>( A )</td>
<td>Depreciation</td>
<td>[$/\text{year}]</td>
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<td>( AUC )</td>
<td>Average costs per unit</td>
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</tr>
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<td>( c )</td>
<td>Capital charge</td>
<td>[-]</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Unit</td>
</tr>
<tr>
<td>--------</td>
<td>--------------------------------------------------</td>
<td>----------</td>
</tr>
<tr>
<td>Co</td>
<td>PE-Plant Cost Index</td>
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</tr>
<tr>
<td>Cf</td>
<td>Complexity factor</td>
<td>[-]</td>
</tr>
<tr>
<td>CF</td>
<td>Cash flow</td>
<td>[$/year]</td>
</tr>
<tr>
<td>C_I</td>
<td>PE-Plant Cost Index</td>
<td>[-]</td>
</tr>
<tr>
<td>C_I</td>
<td>CE-Plant Cost Index</td>
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<td>DCF</td>
<td>Discount Cash Flow</td>
<td>[MS]</td>
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<td>D_i</td>
<td>Discount factor in year i</td>
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<td>f</td>
<td>Costliness index</td>
<td>[-]</td>
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<tr>
<td>f</td>
<td>Investment factor</td>
<td>[-]</td>
</tr>
<tr>
<td>F_m</td>
<td>Material factor</td>
<td>[-]</td>
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<tr>
<td>F_p</td>
<td>Pressure factor</td>
<td>[-]</td>
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<tr>
<td>F_t</td>
<td>Temperature factor</td>
<td>[-]</td>
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<td>I_B</td>
<td>Investments in process units</td>
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<td>Investment costs in fixed capital</td>
<td>[$]</td>
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<tr>
<td>I_h</td>
<td>Investments in auxiliary facilities</td>
<td>[$]</td>
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<tr>
<td>I_e</td>
<td>Investments in miscellaneous capital</td>
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<td>IRR</td>
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<td>[%]</td>
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<td>I_T</td>
<td>Total investment costs</td>
<td>[$]</td>
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<tr>
<td>I_w</td>
<td>Investment costs in working capital</td>
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<tr>
<td>K_p</td>
<td>Production volume related costs</td>
<td>[$/year]</td>
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<td>K_T</td>
<td>Total costs</td>
<td>[$/year]</td>
</tr>
<tr>
<td>L</td>
<td>Operating labour related costs</td>
<td>[$/year]</td>
</tr>
<tr>
<td>n</td>
<td>Plant life</td>
<td>[years]</td>
</tr>
<tr>
<td>N</td>
<td>Number of process steps</td>
<td>[-]</td>
</tr>
<tr>
<td>N</td>
<td>Number of units (except pumps and compressors)</td>
<td>[-]</td>
</tr>
<tr>
<td>N</td>
<td>Number of functional units</td>
<td>[-]</td>
</tr>
<tr>
<td>NCF</td>
<td>Net Cash Flow</td>
<td>[MS]</td>
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<tr>
<td>P</td>
<td>Capacity of the process</td>
<td>[kton/year]</td>
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<td>P_av</td>
<td>Average capacity per unit</td>
<td>[ton/year]</td>
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<tr>
<td>POT</td>
<td>Pay-Out-Time</td>
<td>[years]</td>
</tr>
<tr>
<td>ROI</td>
<td>Return On Investment</td>
<td>[%]</td>
</tr>
<tr>
<td>S_i</td>
<td>Complexity score for a process step</td>
<td>[-]</td>
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<tr>
<td>T</td>
<td>Maximal possible temperature</td>
<td>[K]</td>
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<tr>
<td>V</td>
<td>Total income</td>
<td>[$/year]</td>
</tr>
<tr>
<td>W</td>
<td>Annual profit before taxes</td>
<td>[$/year]</td>
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</tbody>
</table>

FVO 3181 Nomenclature
Appendix A

Original description of the preliminary design project
The preliminary design of a grassroots aromatics complex including a xylene splitter, ortho-xylene column, para-xylene separation unit and a xylene isomerization unit is to be developed for Raytheon Engineers & Constructors, Den Haag.

The xylene splitter, ortho-xylene column and xylene isomerization unit will be designed according to a design basis given by Raytheon Engineers & Constructors. The design does not include the para-xylene separation unit, which will be handled as a black box. In addition the following situation will be studied:

The para-xylene recovery in the para-xylene separation unit will be changed into 95%. This will decrease the para-xylene concentration to the isomerization unit to about 1.5 wt%. The bottlenecks in the designed units will be studied, while the volumetric feed flow to the isomerization unit is maintained.
Appendix B

Process flowsheet
Appendix C

Mass and Heat Balance
### Appendix CI: Mass and heat balance situation 1

<table>
<thead>
<tr>
<th>IN</th>
<th>M (kg/s)</th>
<th>Q (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.51</td>
<td>-35.40</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>forward</th>
<th>M (kg/s)</th>
<th>Q (kW)</th>
</tr>
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<tbody>
<tr>
<td>48.69</td>
<td>-17693.0</td>
<td></td>
</tr>
<tr>
<td>1.20</td>
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<td></td>
</tr>
<tr>
<td>4.29</td>
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</tr>
</tbody>
</table>

| 13.27  | 36955.2  |

<table>
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<th>M (kg/s)</th>
<th>Q (kW)</th>
</tr>
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<tbody>
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<td>33.19</td>
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</tr>
<tr>
<td>-424.68</td>
<td></td>
<td></td>
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</table>

<table>
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<th>OUT</th>
<th>M (kg/s)</th>
<th>Q (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13.27</td>
<td>19953.5</td>
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<tr>
<td>17067.6</td>
<td></td>
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</table>

<table>
<thead>
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<th>transport</th>
<th>M (kg/s)</th>
<th>Q (kW)</th>
</tr>
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<tbody>
<tr>
<td>17.78</td>
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<td></td>
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<tr>
<td>6.97</td>
<td>13.03</td>
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<table>
<thead>
<tr>
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</table>

<table>
<thead>
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<th>Q (kW)</th>
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</thead>
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<td></td>
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</table>

C-1
<table>
<thead>
<tr>
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<th>IN M (kg/s)</th>
<th>Q (kW)</th>
<th>OUT M (kg/s)</th>
<th>Q (kW)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
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**Diagram:**

- T7
- C19
- V29
- H28
- R23
- F20
- H15

**Flow Path:**

- Transport from IN to OUT
- Mass Flow: 39.72 kg/s
- Heat Flow: 91667.0 kW

**Return Path:**

- Mass Flow: 39.72 kg/s
- Heat Flow: 91667.0 kW
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C-4
### Appendix CII: Mass and heat balance situation 2

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### Mass and Heat Balance

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<th>Q (kW)</th>
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<th>M (kg/s)</th>
<th>Q (kW)</th>
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Diagram with flow paths and heat exchanger labeled as:
- H 15
- F 20
- R 23
- H 28
- V 29
- C 19
- T 7
### IN

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### forward

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### return

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### OUT

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**Notes:**
- Mass and Heat Balance
- Forward return
- Transport
- OUT

**Data:**
- M (kg/s): Mass flow rate
- Q (kW): Heat flow rate
- Transport: Mass flow rate and heat flow rate for transport processes.

**Processes:**
- H 18
- H 25
- P 27
- H 17
- V 21
- P 22
- H 24
- P 26

**Values:**
- 5.32 kW
- 4.54 kW
- 6.39 kW
- 5.46 kW
- 1.07 kW
- 0.92 kW
- 2257.82 kW
Appendix D

Stream compositions

In the following tables the compositions, enthalpies, temperatures and pressures of the streams are listed. The following units are used:

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<td>Enthalpy</td>
<td>Mcal/h</td>
<td>Pressure</td>
<td>bar G</td>
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# FVQ 3181 Stream compositions

## DI: Stream compositions situation 1

### Table DI.1: stream compositions of the first situation

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D - 2
FVO 3181 Stream compositions

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### DII : Stream compositions situation 2

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Appendix E

Equipment design

The equipment considered in this appendix was designed using the units of measurement given in different design methods in literature. In the specification forms (Appendix K) all results are given in the requested units.
EI Design of the reactor

The reactor in this process is a fixed bed reactor. Since no kinetic data were available, the volume of the reactor was determined by the liquid hourly space velocity, LHSV. The LHSV is given by equation EI.1, Scott Fogler (1992):

\[ LHSV = \frac{V_{\text{reactor}}}{\Phi_{V,60^\circ F}} \]  

where \( V_{\text{reactor}} \) = volume of the reactor \( \left[ m^3 \right] \)
\( \Phi_{V,60^\circ F} \) = liquified volume stream to the reactor at 60°F \( \left[ m^3/h \right] \)

For the packed bed the actual volume was calculated by dividing the volume obtained from equation EI.1 by the porosity.

The pressure drop over a fixed bed is given by equation:

\[ \frac{\Delta p}{h} = \left( \frac{\rho_g \cdot v^2}{d_p} \right) \cdot \left( \frac{1 - \varepsilon}{\varepsilon^2} \right) \cdot \left( \frac{150 \cdot \varepsilon \cdot \mu}{d_p \cdot r \cdot v} + 1.75 \right) \]  

where \( \Delta p \) = pressure drop \( \left[ \text{Pa} \right] \)
\( h \) = height of the reactor \( \left[ \text{m} \right] \)
\( \rho_g \) = gas density \( \left[ \text{kg/m}^3 \right] \)
\( v \) = superficial velocity \( \left[ \text{m/s} \right] \)
\( d_p \) = diameter of the particles \( \left[ \text{m} \right] \)
\( \varepsilon \) = porosity \( [-] \)
\( \mu \) = viscosity \( \left[ \text{Pa.s} \right] \)

In order to obtain a good fluid distribution in the reactor a fluid distributor is needed. When the height to diameter ratio is low, a low pressure drop is obtained. However the volume of the fluid distributor will be relatively large. This results in higher reactor costs. When the height to diameter ratio is high, the pressure drop will be high. So a height to diameter ratio between these two extremes has to be chosen.
The outlet temperature of the reactor was calculated with a heat balance. Since the reactor is adiabatic the heat balance over the reactor is:

\[
\sum_{i=1}^{n} (x_{i,e} \cdot H_{f,298,i} + \int_{298}^{T_e} x_{i,e} \cdot c_{p,i} \cdot dT) = \sum_{i=1}^{n} (x_{i,o} \cdot H_{f,298,i} + \int_{298}^{T_o} x_{i,o} \cdot c_{p,i} \cdot dT)
\]  

where 
\[n\] = number of components
\[x_{i,e}\] = mol fraction of component i at the reactor entrance
\[H_{f,298,i}\] = enthalpy of formation of component i at 298K
\[T_e\] = temperature at the reactor entrance
\[c_{p,i}\] = heat capacity of component i
\[x_{i,o}\] = mol fraction of component i at the reactor outlet
\[T_o\] = temperature at the reactor outlet

When the mol fractions of all the components at the reactor entrance and outlet are known, and the temperature at the reactor entrance is known the outlet temperature can be calculated.

The given LHSV for this process is 2.5 v/vh. The volume of the liquified feed stream to the reactor at 60 °F, obtained by ChemCadIII, is 58.6 m³/h. Assuming that the porosity of the bed is 0.4 the volume of the reactor, calculated with equation E1.1, is 58.6 m³.

In order to keep the pressure drop low and to prevent a too large volume of the fluid distributor a height to diameter ratio of 1.7 was chosen. So the height of the reactor is 6.0 m and the diameter is 3.5 m. The pressure drop over the reactor, calculated with equation E1.2, then becomes 0.50 bar.

The entrance and outlet mol fraction can be obtained from Appendix D. The entrance temperature is 668.0 K. Equation E1.3 then gives a outlet temperature of 672.0 K.
EII. Design of the distillation columns

The distillation columns were simulated with ChemCadIII. First the number of stages, the feed stage and the reflux ratio were determined with the short cut method. With these results the columns were made rigorous. The (packed) column dimensions and the column pressure drops were calculated with the SULPAK program from the Sulzer company.

The following data were needed by the SULPAK program:

- the number of theoretical stages
- the liquid and gas flows on the top and the bottom stage of each section
- the densities of the gas and liquid streams
- the liquid viscosities and the surface tensions

These data were obtained from ChemCadIII.

Several types of packing could be selected with the SULPAK program. Because of the large streams the 250X packing was chosen. A larger surface area reduces the column size but increases the column pressure drop. Packings with larger surface areas are also more difficult to clean.

The total height of the columns was calculated with the following equation:

\[
    h_{\text{col}} = h_{\text{pb}} + h_x + h_{\text{red}}
\]

where

- \( h_{\text{col}} \) = total column height [m]
- \( h_{\text{pb}} \) = height of the packed bed [m]
- \( h_x \) = height required to remove top and bottom streams [m]
- \( h_{\text{red}} \) = total height required for the redistributors [m]

The height of the packed bed required was obtained from the SULPAK program. From Olujic (1994) it was obtained that redistributors were required after every 15 theoretical stages, to prevent maldistribution.

The height required to remove the top and bottom streams is 6 m.
For the redistributors a height of 2 m per redistributor was chosen.
Example calculation of distillation column T16

First a shortcut calculation in ChemCadIII was made. *ortho-Xylene* was taken as the light key component with a light key split of 0.99 and *cumene* was taken as the heavy key component with a heavy key split of 0.04. The ratio $R/R_{\text{min}}$ was taken as 1.3, a commonly accepted value, which is in general near the economic optimum. The results of this shortcut method were used to make the column rigorous. The most important results were:

- Number of theoretical stages : 77
- Feed entering at stage : 41
- Mass reflux ratio : 5.16

From SULPAK the total height of the packed bed was obtained. This total height was:

$$h_{pb} = 38.5 \text{ m}$$

The feed enters just above stage 41. So above the feed-entrance there are 40 theoretical stages. This part was divided in three packed beds, with respectively 13, 14 and 13 theoretical stages. The bottom part of the column (37 theoretical trays) was divided into three parts of 12, 13 and 12 theoretical stages respectively. Three beds were chosen instead of two to prevent maldistribution. Five redistributors were needed.

The total height of the column was calculated with equation EII.1:

$$h_{col} = 54.5 \text{ m}$$

The diameter of the column was also obtained from SULPAK:

$$D_{col} = 1.288 \text{ m}$$

SULPAK also calculated the pressure drop of the packed beds. The pressure drop varied between 2.8 and 3.0 mbar/m packed bed. The assumption was made that the pressure drop of the liquid redistributors was the same as the pressure drop of the packed beds.

An average pressure drop of 2.9 mbar/m was taken, the total column pressure drop was calculated to be 158 mbar.
EIII Design of the aircoolers

For the condensers of the distillation columns aircoolers were used. The design of the aircoolers was based on the method given by Brown (1978).

From the heat duty obtained from ChemCadIII, the corrected log mean temperature difference and the overall heat transfer coefficient, the hypothetical bare-tube surface can be calculated as:

\[
A = \frac{Q}{U \cdot \Delta T_{\text{lm,cor}}}
\]

where
- \(A\) = hypothetical bare-tube surface [\(\text{ft}^2\)]
- \(Q\) = heat duty [\(\text{Btu/h}\)]
- \(U\) = overall heat transfer coefficient [\(\text{Btu/h/ft}^2/\text{°F}\)]
- \(\Delta T_{\text{lm,cor}}\) = corrected log mean temperature difference [\(\text{°F}\)]

The overall heat transfer coefficient can be found in literature.

The corrected log mean temperature difference was calculated with the following equation:

\[
\Delta T_{\text{lm,cor}} = c_{fm_{TD}} \cdot \Delta T_{\text{lm}}
\]

where
- \(c_{fm_{TD}}\) = mean temperature difference correction factor [-]
- \(\Delta T_{\text{lm}}\) = log mean temperature difference [\(\text{°F}\)]

The log mean temperature difference is:

\[
\Delta T_{\text{lm}} = \frac{\Delta t_2 - \Delta t_1}{\ln(\Delta t_2/\Delta t_1)}
\]

where
- \(\Delta t_2\) = greatest temperature difference at inlet or outlet [\(\text{°F}\)]
- \(\Delta t_1\) = least temperature difference at inlet or outlet [\(\text{°F}\)]

As the condenser only condenses the fluid, and is not used as a cooler, it is assumed that the inlet temperature equals the outlet temperature.

The inlet air temperature was specified as the air temperature that is not exceeded during 98 % of the year.

The exit air temperature was calculated as:

\[
t_2 = t_1 + 0.005 \cdot U \cdot \left[\frac{(T_2 + T_1)}{2} - t_1\right]
\]

where
- \(t_1\) = inlet air temperature [\(\text{°F}\)]
- \(t_2\) = outlet air temperature [\(\text{°F}\)]
- \(T_1\) = outlet fluid temperature [\(\text{°F}\)]
- \(T_2\) = inlet fluid temperature [\(\text{°F}\)]
The mean temperature difference correction factor was obtained from Figure 2, Brown (1978), by using the temperature efficiency and the correlating factor:

\[ R = \frac{(T_2 - T_1)}{(t_2 - t_1)} \]  

where \( R \) = correlating factor  

The temperature efficiency is defined as:

\[ P = \frac{(t_2 - t_1)}{(T_2 - T_1)} \]  

where \( P \) = temperature efficiency  

With the calculated bare-tube surface, see equation EIII.1, the unit size can be defined from Table II, Brown (1978).

To calculate the pressure drop through the condenser tubes, the pressure drop for a total gas flow was calculated and divided by two, to account for the mixed phase flow.

The pressure drop for a gas flow is defined by:

\[ \Delta P = 6 \cdot j_f \cdot \left( \frac{L_{\text{hydrate}}}{D_t} \right) \cdot \left( \frac{\rho_{\text{gas}} \cdot v_{\text{gas}}^2}{2} \right) \]  

where \( \Delta P \) = pressure drop for total gas flow  
\( j_f \) = friction factor  
\( L_{\text{hydrate}} \) = hydraulic length  
\( D_t \) = tube inner diameter  
\( \rho_{\text{gas}} \) = fluid gas density  
\( v_{\text{gas}} \) = fluid gas velocity

The friction factor was found from Figure 12.24, Sinnott (1993), as a function of the Reynolds number.  
The hydraulic length is equal to the tube length.
The gas velocity through the tubes is equal to:

\[ v_{\text{gas}} = \frac{\dot{m}}{\rho_{\text{gas}} \cdot A_{\text{cross}}} \]  

where \( \dot{m} \) = fluid mass flow \([\text{lb/s}]\)  
\( \rho_{\text{gas}} \) = total cross section of the tubes \([\text{ft}^2]\)

According to Sinnott (1993) the gas velocity should have a value between 10-30 \( \text{m/s} \).
To define the total cross section, the total number of tubes was needed:

\[ n_{t,\text{total}} = \frac{A}{A_{\text{tube}}} \]  

where \( n_{t,\text{total}} \) = total number of tubes \([-]\)  
\( A \) = total bare tube surface \([\text{ft}^2]\)  
\( A_{\text{tube}} \) = surface of one tube \([\text{ft}^2]\)

Finally, the pressure drop through the condenser tubes was calculated for the mixed flow by dividing the pressure drop for total gas flow by two.
Example calculation of aircooler H2

The heat duty obtained from ChemCad III for aircooler H2 was -58.02 MBtu/h. The overall heat transfer coefficient obtained from Brown (1978) was: \( U = 50 \) Btu/h/ft\(^2\)°F.

The average fluid temperature was 282.3 °F. The inlet air temperature was 98.6 °F (37 °C). By using equation EIII.3, the exit air temperature was calculated and was 144.5 °F. The temperature differences were:

\[
\begin{align*}
\Delta t_1 &= 183.7 \degree F \\
\Delta t_2 &= 137.8 \degree F 
\end{align*}
\]

The log mean temperature difference was calculated with equation EIII.2:

\[ \Delta t_{lm} = 159.6 \degree F \]

The temperature efficiency was 0.25, and the correlating factor was 0 (see equations EIII.6 and EIII.5). From Figure 2, Brown (1978), the MTD correction factor was found to be: \( c_{MTD} = 1.00 \). Then, according to equation EIII.4, the corrected log mean temperature difference was 159.6°F.

The hypothetical bare tube surface was calculated with equation EIII.1:

\[ A = 7269 \text{ ft}^2 \]

Six units of 12 ft wide with three rows of 30-ft-long tubes for a total bare tube surface of 7734 ft were chosen (see Table II, Brown (1978)), to keep the gas velocity within the specified range. The surface of one tube was 7.85 ft\(^2\), so the total number of tubes required was 985 (equation EIII.9), for a total cross section of 5.37 ft\(^2\). As the flow through the tubes was 106.96 lb/s, and the gas density was 0.2090 lb/ft\(^3\), the gas velocity was 95.3 ft/s, according to equation EIII.8.

The Reynolds number was 2.55\( \times 10^4 \), so the friction factor was 2.0\( \times 10^{-3} \), from Figure 12.24 Sinnott (1993). The hydraulic length was equal to the tube length: \( L_{hyd} = 12 \) ft.

The pressure drop for total gas flow was calculated with equation EIII.7, and was 1.36 psi. For the mixed flow, the total pressure drop was 0.681 psi, or 47 mbar.
EIV Design of the heat exchangers

The heat transfer equipment was designed according to the methods described by Sinnott (1993).

The general equation for heat transfer across a surface is:

\[ Q = U \cdot A \cdot \Delta T_m \]  

where:
- \( Q \) = heat transfer per unit time \([\text{W}]\)
- \( U \) = overall heat transfer coefficient \([\text{W/m}^2\text{°C}]\)
- \( A \) = heat-transfer area \([\text{m}^2]\)
- \( \Delta T_m \) = mean temperature difference \([\text{°C}]\)

The overall coefficient is the reciprocal of the overall resistance to heat transfer, which is the sum of several individual resistances. For heat exchange across a typical heat-exchanger tube the relationship between the overall coefficient and the individual coefficients is given by:

\[ \frac{1}{U} = \frac{1}{h_o} + \frac{1}{h_{i d}} + \frac{d_i \ln(d_i/d_o)}{2k_w} + \frac{d_i}{d_o} \left( \frac{1}{h_{i d}} - \frac{1}{h_i} \right) \]  

where:
- \( h_o \) = outside fluid film coefficient \([\text{W/m}^2\text{°C}]\)
- \( h_i \) = inside fluid film coefficient \([\text{W/m}^2\text{°C}]\)
- \( h_{i d} \) = outside dirt coefficient (fouling factor) \([\text{W/m}^2\text{°C}]\)
- \( h_{i d} \) = inside dirt coefficient \([\text{W/m}^2\text{°C}]\)
- \( k_w \) = thermal conductivity of the tube wall material \([\text{W/m}^2\text{°C}]\)
- \( d_i \) = tube inner diameter \([\text{m}]\)
- \( d_o \) = tube outer diameter \([\text{m}]\)

A first estimate of the overall heat transfer coefficient was obtained from Table 12.1, Sinnott (1993).

The mean temperature difference, \( \Delta T_m \), can be calculated from the logarithmic mean temperature difference by applying a correction factor to allow for the departure from true counter-current flow:

\[ \Delta T_m = F_t \cdot \Delta T_{lm} \]  

where:
- \( F_t \) = temperature correction factor \([-]\)
- \( \Delta T_{lm} \) = log mean temperature difference \([\text{°C}]\)
The logarithmic mean temperature difference is given by:

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

where

- \( T_1 \) = inlet shell-side temperature [°C]
- \( T_2 \) = outlet shell-side temperature [°C]
- \( t_1 \) = inlet tube-side temperature [°C]
- \( t_2 \) = outlet tube-side temperature [°C]

The correction factor is a function of the shell- and tube-side fluid temperatures, and the number of tube and shell passes. It is normally correlated as a function of two dimensionless temperature ratios:

$$R = \frac{T_1 - T_2}{t_2 - t_1}$$  EIV.5

$$S = \frac{t_2 - t_1}{T_1 - t_1}$$  EIV.6

The correction factor as a function of these two dimensionless ratios is given in Figures 12.19-12.22, Sinnott (1993), for different heat exchanger configurations.

When \( Q, U \) and \( \Delta T_m \) are determined the area needed can be calculated from equation EIV.1. The number of tubes can be calculated by dividing the total area by the area of one tube.

The area of one tube is:

$$A_t = \pi \cdot d_o \cdot L$$  EIV.7

where

- \( A_t \) = area of one tube \( [\text{m}^2] \)
- \( L \) = length of the tube \( [\text{m}] \)

The layout of the exchanger and the dimensions of the tubes were selected in such a way that the velocities and pressure drops remained within the specified limits. For the shell and tube exchangers the tube length to shell diameter ratio should also be in the range of 5 to 10. This is the economical optimum according to Sinnott (1993). The tubes were arranged in an equilateral triangular pattern, because of the higher heat transfer rates compared with a square pattern. The tube pitch is chosen as 1.25 times the tube outside diameter. Because of the high temperature differences exchangers with an internal floating head were used.

The tube-side velocity can be determined by dividing the volumetric flow on the tube side by the available cross-sectional area per pass.
The bundle diameter will depend on the number of tubes and also on the number of tube passes, as spaces must be left in the pattern of tubes on the tube sheet to accommodate the pass partition plates. The bundle diameter was calculated with:

\[ D_b = d_o \cdot \left( \frac{N_t}{K_i} \right)^{\frac{1}{n_i}} \]

where
- \( D_b \) = bundle diameter [m]
- \( N_t \) = number of tubes [-]
- \( K_i \) = constant [-]
- \( n_i \) = constant [-]

The constants \((K_i\) and \(n_i\)) are given in Table 12.4, Sinnot (1993).

The shell diameter can be determined by adding a shell-bundle clearance to the bundle diameter. The clearance required depends on the type of heat exchanger used and can be obtained from Figure 12.10, Sinnot (1993).

For the tubes and shells of the heat exchangers carbon steel will be used. The corrosion chart in Sinnot (1993) indicates that this material is resistant to water and the organic mixture at the given process conditions. The conductivity of carbon steel at the process conditions is taken as \( k_w = 50 \text{ W/m}^2\text{C}\). For the fouling factors the following values were used:

- water : 931.1 \( \text{W/m}^2\text{C}\)
- organic mixture : 5819 \( \text{W/m}^2\text{C}\)

**Vaporiser**

In the heat exchanger H15 the reactor outlet stream is used to pre-heat the reactor inlet stream. The reactor outlet stream is fed to a gas-liquid separator. This separator gives a better separation at a higher pressure. Because the tube-side pressure drop is lower than the shell-side pressure drop, the reactor outlet stream is allocated in the tubes. The reactor outlet stream is a vapour, the inlet stream at the shell side of heat exchanger H15 is a vapour/liquid mixture.

The tube-side heat transfer coefficient is defined by:

\[ h_t = \frac{j_h \cdot k_f}{d_i} \cdot Re \cdot Pr^{0.33} \]

where
- \( j_h \) = heat transfer factor [-]
- \( k_f \) = thermal conductivity \( \text{W/m}^2\text{C}\)
- \( Re \) = Reynolds number [-]
- \( Pr \) = Prandtl number [-]

The heat transfer factor \((j_h)\) was obtained from Figure 12.23, Sinnot (1993).
The tube-side pressure drop was calculated by:

$$\Delta P_t = N_p \cdot (8 \cdot \text{j}_r \cdot (L / d_t) + 2.5) \cdot \left( \frac{\rho \cdot u_t^2}{2} \right)$$  \hspace{1cm} \text{EIV.10}$$

where:
- $\Delta P_t$ = tube-side pressure drop [N/m$^2$]
- $N_p$ = number of tube-side passes [-]
- $\text{j}_r$ = friction factor [-]
- $\rho$ = density of fluid [kg/m$^3$]
- $u_t$ = tube-side velocity [m/s]

The friction factor was read from Figure 12.24, Sinnot (1993).

The reactor inlet stream at the shell-side is totally vaporized. During the vaporization two types of boiling will occur: nucleate boiling and convective boiling. At low temperature differences, when the liquid is below its boiling point, heat is transferred by natural convection. As the surface temperature is increased incipient boiling occurs, vapour bubbles forming and breaking loose from the surface. The agitation caused by the rising bubbles, and the other effects caused by bubble generation at the surface, result in a large increase in the rate of heat transfer. This phenomenon is known as nucleate boiling. To estimate the effective heat transfer coefficient Chen’s method (Sinnot (1993)) was used:

$$h_e = h_f c \cdot f_c \cdot h_{nb} \cdot f_n$$  \hspace{1cm} \text{EIV.11}$$

where:
- $h_e$ = effective outside heat-transfer coefficient [W/m$^2$/°C]
- $h_f c$ = forced convection coefficient assuming liquid fase is in conduit alone [W/m$^2$/°C]
- $f_c$ = factor to account for the effects of two-phase flow [-]
- $h_{nb}$ = nucleate boiling coefficient [W/m$^2$/°C]
- $f_n$ = factor to account for the fact that nucleate boiling is more difficult in a flowing liquid [-]

The coefficient for convective boiling was calculated by:

$$h_f c = \frac{j b \cdot k_f}{d_e} \cdot Re_L \cdot Pr^{1/3}$$  \hspace{1cm} \text{EIV.12}$$

where:
- $d_e$ = equivalent diameter [m]
- $Re_L$ = liquid Reynolds number [-]

The value of $j b$ was read from Figure 12.29, Sinnot (1993).

The liquid Reynolds number is given by:

$$Re_L = \frac{(1 - x) \cdot G \cdot d_e}{\mu_L}$$  \hspace{1cm} \text{EIV.13}$$

where:
- $G$ = total mass flow rate per unit flow area [kg/m$^2$/s]
- $d_e$ = equivalent diameter [m]
- $\mu_L$ = liquid viscosity [N·s/m$^2$]
- $x$ = mass fraction of vapour [-]
The area for cross-flow at the shell equator is given by:

\[ A_s = \frac{(p_t - d_{in}) \cdot D_s \cdot l_b}{p_t} \]  

where \( A_s \) = cross-flow area [m²], 
\( p_t \) = tube pitch [m], 
\( D_s \) = shell diameter [m], 
\( l_b \) = baffle spacing [m].

For an equilateral triangular pitch arrangement the equivalent diameter is:

\[ d_e = \frac{1.10}{d_o} \cdot (p_t^2 - 0.917 \cdot d_o^2) \]  

For the mass fraction of vapor the average between the inlet and outlet value was taken as a good estimate for the preliminary design.

With the Lockhart-Martinelli two-phase flow parameter the two-phase correction factor \( f_c \) was obtained from Figure 12.56, Sinnot (1993). The Lockhart-Martinelli two-phase flow parameter with turbulent flow in both phases is defined as:

\[ \frac{1}{X_{nt}} = \frac{1 - x}{x} \cdot \left( \frac{\rho_L}{\rho_v} \right)^{0.5} \cdot \left( \frac{\mu_v}{\mu_L} \right)^{0.1} \]  

where \( 1/X_{nt} \) = Lockhart-Martinelli two-phase flow parameter [-], 
\( x \) = mass fraction of vapor [-], 
\( \rho_L \) = liquid density [kg/m³], 
\( \rho_v \) = vapor density [kg/m³], 
\( \mu_v \) = vapor viscosity [N·s/m²], 
\( \mu_L \) = liquid viscosity [N·s/m²].

The nucleate boiling coefficient is estimated using the Mostinski correlation:

\[ h_{nb} = 0.104 \cdot (P)^{0.69} \cdot (q)^{0.7} \cdot \left( 1.8 \cdot (P/P_c)^{0.17} + 4 \cdot (P/P_c)^{1.2} + 10 \cdot (P/P_c)^{10} \right) \]  

where \( P \) = the operating pressure [bar], 
\( P_c \) = the liquid critical pressure [bar], 
\( q \) = heat flux [W/m²].

It is recommended that the heat flux in thermosyphon reboilers, based on the total heat transfer area, should not exceed a critical value. At this critical flux, the rate of vapor generation is such that dry patches occur spontaneously over the surface, and the rate of heat transfer falls off rapidly.

The suppression factor \( f_s \) was obtained from Figure 12.57, Sinnot (1993).
The pressure drop on the shell-side was calculated from:

$$\Delta P_s = 8 \cdot f_r \cdot \left( \frac{D_s}{d_t} \right) \cdot \left( \frac{L}{l_o} \right) \cdot \frac{\rho_s \cdot u_s^2}{2}$$  

where
- $\Delta P_s$ = pressure drop on the shell-side  
- $u_s$ = shell-side velocity

### Condenser

The heat exchanger H28 is used to cool the outlet reactor stream before it enters the gas/liquid separator. To cool the outlet reactor stream cooling water is used. The cooling water flows through the tubes. The condensation is in the shell-side.

For the tube-side heat transfer coefficient Eagle and Ferguson give an equation specifically developed for water:

$$h_t = 4200 \cdot (1.35 + 0.02 \cdot t) \cdot u_t^{0.8} / d_t^{0.2}$$

where
- $t$ = water temperature  
- $u_t$ = water velocity

The pressure drop on the tube-side was calculated with equation EIV.10.

The shell-side heat transfer coefficient was determined, using Kern's method (Sinnott 1993). This model assumes total condensation. As 75 wt% of the process stream condenses, this model was used to obtain a rough estimate for the shell-side heat transfer coefficient. Using Kern's method, the mean coefficient for a tube bundle is given by:

$$h_o = 0.95 \cdot k_L \cdot \left[ \frac{\rho_L \cdot (\rho_L - \rho_v) \cdot g \cdot \Gamma_h}{\mu_L \cdot \Gamma_h} \right]^{1/3} \cdot N_t^{-1/6}$$

where
- $k_L$ = condensate thermal conductivity  
- $\rho_L$ = condensate density  
- $\rho_v$ = vapour density  
- $\mu_L$ = condensate viscosity  
- $g$ = gravitational acceleration  
- $\Gamma_h$ = tube loading  
- $N_t$ = average number of tubes in a vertical tube row

The tube loading is given by:

$$\Gamma_h = \frac{W_c}{L \cdot N_t}$$

where
- $W_c$ = total condensate flow  
- $L$ = tube length  
- $N_t$ = total number of tubes in the bundle
For the condensate a mean temperature was estimated by taking the average of the wall temperature and the mean shell-side temperature. The wall temperature, in turn, was estimated by assuming a shell-side condensing coefficient and an overall coefficient and using the following equation:

\[ h_n \cdot (T - T_w) = U \cdot (T - t) \]  

EIV.22

where
- \( T_w \) = wall temperature [°C]
- \( T \) = mean shell-side temperature [°C]
- \( t \) = mean tube-side temperature [°C]

This is an iterative process.

The shell-side pressure drop was determined by equation EIV.18, using the inlet vapour conditions and applying a correction factor of 0.5, suggested by Kern.

**Reboilers**

For the reboilers thermosyphon reboilers were used. The liquid circulation through the exchanger is maintained by the difference in density between the two-phase mixture of vapour and liquid in the exchanger and the single-phase liquid in the base of the column. Horizontal thermosyphon reboilers were used because these are easier to clean than vertical thermosyphon reboilers. Another reason is that for horizontal reboilers the steam flows through the tubes. This way no expensive pressure resistant shell wall is required. Medium pressure steam is used for all three reboilers. The steam is in the tubes, the process fluid in the shell.

For the design of a thermosyphon reboiler for a distillation column the following data are required:

- Boiling point of the liquid at the bottom-pressure of the column
- Critical temperature of the liquid at the base of the column
- Steam saturation temperature
- Heat load

The mean overall temperature difference was calculated by:

\[ \Delta T_{m} = T_{sat} - T_{b} \]  

EIV.23

where
- \( \Delta T_{m} \) = mean overall temperature difference [°C]
- \( T_{sat} \) = steam saturation temperature [°C]
- \( T_{b} \) = boiling temperature of liquid at bottom-pressure [°C]

From Figure 12.59 in Sinnott (1993) the design heat flux for a vertical thermosyphon reboiler can be obtained as a function of \( \Delta T_{m} \) and the reduced temperature (\( T_r \)). This Figure was also used for the design of the horizontal reboilers.
The required area can be obtained by dividing the heat load by the design heat flux:

\[ A = \frac{Q}{Q''} \]  

EIV.24

where

- \( A \) = area required \([m^2]\)
- \( Q \) = heat load \([kW]\)
- \( Q'' \) = heat flux \([kW/m^2]\)

By dividing the required area by the area of one tube the number of tubes required can be obtained. The diameter of the bundle and the shell clearance were determined the same way as done for the heat exchangers (equation EIV.8).

The top tube sheet is normally aligned with the liquid level in the base of the column. The outlet pipe should have a cross-sectional area at least equal to the total cross-sectional area of the shell-side. The outlet pipe diameter was calculated by:

\[ D_p = \sqrt{N_i \cdot d_i^2} \]  

EIV.25

where

- \( D_p \) = outlet pipe diameter \([m]\)
- \( N_i \) = number of tubes \([-]\)
- \( d_i \) = inside-tube diameter \([m]\)

The shell-side pressure drop was calculated with equation EIV.18. This was done for the inlet conditions and for the outlet conditions of the reboiler. The average of both values was taken as a good estimate. The pressure drop for the steam (tube-side) was obtained from equation EIV.10.

For all heat exchangers a 10% larger heat transfer area was installed to anticipate for future expansions.
Example calculation of heat exchanger H28

As an example for the design of a shell and tube heat exchanger the condenser (H28) calculation will be demonstrated.

The calculation of the overall heat transfer coefficient is an iterative process.

The organic mixture was cooled from 193.1 K to 48.9 °C.
The total flow was 66,204 kg/h.
The heat duty obtained by ChemCadIII was 10,930 kW.
The cooling water was allowed to heat up from 27 °C to 30 °C.

The required cooling water flow was obtained by dividing the heat duty by the heat capacity of water and the allowed heat-up of the cooling water.

\[
\text{With } \frac{c_p \cdot w}{\Delta T} = 4.178 \text{ kJ/kg} \cdot \text{°C} \quad \Delta T = 7 \text{ °C}
\]

it was calculated that the required cooling water flow was 373.7 kg/s = 1,345 ton/h.

With equations EIV.3-EIV.6 the mean temperature difference was obtained:

\[
\Delta T_m = 69.3 \text{ °C} \\
R = 20.6 \\
S = 0.042 \\
F_i = 0.99 \\
\Delta T_m = 68.6 \text{ °C}
\]

For the calculation the overall coefficient, \( U \), had to be estimated.
After several iterations the overall transfer coefficient was found to be:

\( U = 412 \text{ W/m}^2 \cdot \text{°C} \).

The heat transfer area was calculated with equation EIV.1 and was:

\( A = 386.5 \text{ m}^2 \).

For the heat-exchanger the following tube dimensions were selected, in order to keep the velocities and pressure drops within the allowable ranges (for ranges see Sinnott (1993)):

\( d_o = 30 \text{ mm} \)
\( d_i = 26 \text{ mm (2mm tube wall)} \)
\( L = 6.1 \text{ m} \)

The area of one tube is \( \pi \cdot d_i \cdot L = 0.57 \text{ m}^2 \).
The number of tubes required was obtained by dividing the total area by the area of one tube:

\( N_i = 386.5/0.57 = 673 \)
To keep the velocity and the pressure drop on the tube-side within the ranges mentioned by Sinnott (1993) there are two tube passes, so the number of tubes per pass is 337.

The tube-side velocity was calculated by dividing the volumetric flow by the cross-sectional area available per pass, where:

\[ \text{area per pass} = 0.191 \text{ m}^2 \]
\[ \text{water density} = 993.9 \text{ kg/m}^3 \]
\[ u_t = 2.10 \text{ m/s} \quad \text{within 1.5 - 2.5 m/s, Sinnott (1993)} \]

The bundle diameter was calculated with equation EIV.8:
For a triangular tube pitch and two tube passes the constants, \(K_i\) and \(n_1\), are:
\[ K_i = 0.249 \]
\[ n_1 = 2.207 \]

The diameter of the bundle then becomes:
\[ D_b = 1076.7 \text{ mm} \]

For a floating head heat exchanger of this size a shell clearance of 75 mm is required (Figure 12.10, Sinnott (1993)), so the shell diameter is:
\[ D_s = 1076.7 + 75 = 1151.7 \text{ mm} \]

The tube-side heat transfer coefficient was obtained from equation EIV.19:
\[ h_t = 7720.0 \text{ W/m}^2\text{°C} \]

The tube-side pressure drop was calculated with equation EIV.10, with a friction factor of 3\(\cdot10^{-3}\):
\[ \Delta P_t = 0.36 \text{ bar} \]

Before the shell-side condensing coefficient (\(h_o\)) could be determined the mean condensate temperature had to be estimated. The estimation after several iterations was:
\[ h_o = 1217 \text{ W/m}^2\text{°C} \]

From equation EIV.22 a wall temperature of \(T_w = 363.4 \text{ K} \) followed. The mean condensate temperature is the average of the wall temperature and the mean shell-side temperature:
\[ <T_s> = 378.8 \text{ K} \]

The physical properties of the condensate and vapour were obtained from ChemCadIII:
\[ \rho_L = 774 \text{ kg/m}^3 \]
\[ \rho_v = 3.78 \text{ kg/m}^3 \text{ (at mean vapour temperature)} \]
\[ \mu_L = 0.269 \text{ mPa/s} \]
The total condensate flow was also obtained from ChemCadIII and was:

\[ W_c = 13.01 \text{ kg/s}. \]

The average number of tubes in a row is \( \frac{2}{3} \) times the number of tubes in the centre row. For a triangular tube pitch of \( p_t = 1.25 \cdot d_o \), the number of tubes in the centre row is:

\[ N_{\text{centre row}} = \frac{D_s}{p_t} = 28. \]

The shell-side heat transfer coefficient was calculated with equation EIV.20:

\[ h_s = 1217.03 \text{ W/m}^2\text{/°C}. \]

The shell-side pressure drop was determined with equation EIV.18 using the inlet vapour conditions and applying a correction factor of 0.5.

The inlet vapour velocity was obtained by dividing the inlet mass flow by the inlet vapour density and the area for cross flow. The former two were obtained for ChemCadIII, the latter by equation EIV.14.

\[ u_i = 11.7 \text{ m/s} \quad \text{within 10 - 30 m/s, Sinnott (1993)} \]

The equivalent diameter was calculated with equation EIV.15:

\[ d_e = 21.3 \text{ mm}. \]

The baffle spacing \( l_b \) for the condensor was taken as \( l_b = D_s \), and the baffle cut was 0.45. These values were chosen to prevent a high pressure drop on the shell-side. The pressure drop on the shell-side was calculated with equation EIV.18. The friction factor was \( 2.1 \cdot 10^{-2} \).

\[ \Delta P_s = 0.097 \text{ bar}. \]

The overall coefficient could now be calculated, with:

\[ k_w = 50 \quad \text{W/m}^2\text{/°C} \]
\[ h_{ot} = 5819 \quad \text{W/m}^2\text{/°C} \]
\[ h_{id} = 931.1 \quad \text{W/m}^2\text{/°C} \]

equation EIV.2 gives: \[ U = 412.8 \text{ W/m}^2\text{/°C} \]

The new values for \( h_s \) and for \( U \) are close enough to the former estimates. The iteration process has converged.
EV  Design of the fired heater

The design of the fired heater was based on the method described by Berman (1978). Because in this article British units are used the entire calculation is in British units and the final results will be converted to the units used in the rest of this report.

The heater is divided in a radiation section and a convection section. The process fluid enters the heater in the convection section and leaves the heater after the radiation section. The lowest three tube rows in the convection section are called the shield bank. These tubes contribute partly to the radiative heat transfer. The other tubes in the convection section are called the fin bank. Since convection section surface-area requirements are controlled by film resistance it is useful to extend the surface with fins, to improve the heat transfer.

The heat fired was calculated with equation EV.1:

$$Q_f = \frac{Q_a}{\eta}$$  

where  

- $Q_f$ = total heat fired  
- $Q_a$ = heat absorbed by process fluid  
- $\eta$ = efficiency

The efficiency was calculated with equation EV.2

$$\eta = \frac{H_{a,FGT}}{LHV_{fuel}} \cdot 100\% - f_{rl}$$  

where  

- $H_{a,FGT}$ = heat available at the flue gas temperature  
- $LHV_{fuel}$ = liquid heating value of the fuel  
- $f_{rl}$ = fraction radiative loss

The flue gas temperature was estimated to be the temperature of the feed to the heater plus 150 F, as stated by Berman (1978). The radiative loss is generally assumed to be 2% of the fired heat.

The fluid velocity in the tubes was calculated by:

$$v = \frac{\phi_m}{np \cdot \frac{\pi}{4} \cdot D_i^2}$$  

where  

- $v$ = fluid velocity  
- $\phi_m$ = fluid mass flow  
- $np$ = number of passes  
- $D_i$ = inner diameter of the tubes

Note that the number of passes of a fired heater has a different definition than for an unfired heater. At
a fired heater the number of passes is the number of parallel streams. The fluid velocity in the tubes should be between 30 and 90 ft/s for gases, Sinnott (1992). In order to calculate the heat duty of the radiant section, the average bridgework temperature had to be determined. This temperature is given as a function of the average tube metal temperature and the average radiant rate in Figure 6a, Berman (1978).

The radiant heat duty was calculated by:

$$ Q_{\text{rad}} = Q_{\text{a}} \cdot \frac{H_{\text{a,BWT}}}{H_{\text{a,FGT}}} $$

where $Q_{\text{rad}}$ = radiant section heat duty [Btu/h]
$H_{\text{a,BWT}}$ = heat available at the bridgework temperature [Btu/lb]

The total radiant surface was calculated by:

$$ A_{\text{rad}} = \frac{Q_{\text{rad}}}{q_{r}} $$

where $A_{\text{rad}}$ = radiant section surface [ft²]
$q_{r}$ = average radiant rate [Btu/h/ft²]

The surface of one shield row is considered to be part of the radiant surface, so the surface of a shield row should be calculated in order to calculate the length of a radiant tube. The surface of one shield row is:

$$ A_{\text{sh}} = n_{sr} \cdot l_{sh} \cdot \pi \cdot D_{o} $$

where $A_{\text{sh}}$ = surface area of one shield row [ft²]
$n_{sr}$ = number of tubes per shield row [-]
$l_{sh}$ = effective length of one shield row [ft]
$D_{o}$ = outer tube diameter [ft]

The tubes in the radiant section are placed in a circle with a burner in the middle. The maximum length of shield row is determined by the radiant tube circle diameter.

The length of a tube in the radiant section was calculated by equation EV.7.

$$ l_{\text{rad}} = \frac{A_{\text{rad}} - A_{\text{sh}}}{n_{sr} \cdot \pi \cdot D_{o}} $$

where $l_{\text{rad}}$ = length of a tube in the radiant section [ft]
$n_{sr}$ = number of tubes in the radiant section [-]
The calculation of the temperatures and the heat transfer in the shield bank is an iterative process. An assumption has to be made about the flue gas temperature above the shield bank. This assumption has to be checked later on.

The heat transfer in the shield bank was calculated by the well known equation:

\[ Q = U \cdot A \cdot \Delta T_{LM} \]  

where \( Q \) = transferred heat \[ \text{[Btu/h]} \]
\( U \) = overall heat transfer coefficient \[ \text{[Btu/h \cdot ft^2 \cdot °F]} \]
\( A \) = heat transfer area \[ \text{[ft^2]} \]
\( \Delta T_{LM} \) = log mean temperature difference \[ \text{[°F]} \]

The overall heat transfer coefficient was calculated by:

\[ U = \frac{1}{R_0 + R_w + R_i} \]  

where \( R_0 \) = external film resistance \[ \text{[h \cdot ft^2 \cdot °F/Btu]} \]
\( R_w \) = tube-wall resistance \[ \text{[h \cdot ft^2 \cdot °F/Btu]} \]
\( R_i \) = in-tube film resistance \[ \text{[h \cdot ft^2 \cdot °F/Btu]} \]

The external film resistance was calculated by:

\[ R_0 = \frac{1}{1.1 \cdot (h_c + h_{rg})} \]  

where \( h_c \) = convection film coefficient \[ \text{[Btu/h \cdot ft^2 \cdot °F]} \]
\( h_{rg} \) = gas radiation coefficient \[ \text{[Btu/h \cdot ft^2 \cdot °F]} \]

The convection film coefficient was calculated with equation EV.11:

\[ h_c = 2.14 \cdot \frac{G_{fg}^{0.5} \cdot T_{fga}^{0.28}}{D_w^{0.4}} \]  

where \( G_{fg} \) = flue gas mass velocity \[ \text{[lb/s/ft^2]} \]
\( T_{fga} \) = average flue gas temperature \[ \text{[°R]} \]

The gas radiation coefficient was obtained from equation EV.12:

\[ h_{rg} = 0.0025 \cdot T_{fg} - 0.5 \]  

where \( T_{fg} \) = flue gas temperature \[ \text{[°F]} \]
The tube-wall resistance was calculated by:

\[ R_w = \frac{A_o}{h_w \cdot A_i} \]  

where 
- \( A_o \) = external tube surface 
- \( h_w \) = tube wall coefficient 
- \( A_i \) = internal tube surface

The tube-wall coefficient was calculated by:

\[ h_w = \frac{K_m}{t_m} \]  

where 
- \( K_m \) = thermal conductivity of the wall 
- \( t_m \) = thickness of the tube wall

The in-tube film resistance was calculated by:

\[ R_i = \frac{A_o}{h_i \cdot A_i} \]  

where \( h_i \) = in-tube film coefficient

The in-tube film coefficient was calculated with the well known Nusselt relation:

\[ h_i = 0.027 \cdot \frac{k}{D_o} \cdot \left( \frac{D_o \cdot G}{\mu} \right)^{0.8} \cdot \left( \frac{c_p \cdot \mu}{k} \right)^{0.333} \]  

where 
- \( k \) = thermal conductivity of the flue gas 
- \( G \) = fluid mass velocity 
- \( \mu \) = viscosity of the fluid 
- \( c_p \) = specific heat of the fluid

Now the log mean temperature difference over the shield bank can be calculated. The product of the overall heat transfer coefficient, the log mean temperature difference and the total surface of the shield bank gives the shield bank absorption rate.
The heat available at the shield bank temperature was calculated with:

\[
\frac{H_{a,BWT}}{H_{a,s}} = \frac{Q_r}{Q_r + Q_s}
\]

\[\text{EV.17}\]

where \( H_{a,s} \) = heat available at shield bank \[\text{[Btu/lb]}\]  
\( Q_r \) = convective heat duty of the shield bank \[\text{[Btu/lb]}\]

Now the flue gas temperature above the shield bank has to be checked. From Figure 3, Berman (1978), the flue gas temperature was derived. This temperature has to correspond to the assumed value of the flue gas temperature. The heat duty of the fin bank was calculated by:

\[
Q_f = Q_a - Q_r - Q_s
\]

\[\text{EV.18}\]

where \( Q_f \) = heat duty of the fin bank \[\text{[Btu/h]}\]

The method to calculate the heat transfer coefficient for the fin bank is the same as the method for the shield bank with one exception. Equation EV.11 changes in equation EV.19.

\[
h_c = \frac{J \cdot c_p \cdot G}{Re^2} \cdot \left( \frac{E \cdot A_f + A_0}{A_t} \right)
\]

\[\text{EV.19}\]

where \( J \) = heat transfer factor \[\text{[-]}\]  
\( E \) = fin efficiency \[\text{[-]}\]  
\( A_f \) = fin surface of extended-surface tube \[\text{[ft}^2/\text{ft]}\]  
\( Re \) = Reynolds number \[\text{[-]}\]  
\( A_t \) = total surface of finned tube \[\text{[ft}^2/\text{ft]}\]

The number of finned rows was calculated by:

\[
nr = \frac{A_{fb}}{A_{fr}}
\]

\[\text{EV.20}\]

where \( nr \) = number of finned rows \[\text{[-]}\]  
\( A_{fb} \) = surface area of the fin bank \[\text{[ft}^2]\]  
\( A_{fr} \) = surface area of one finned row \[\text{[ft}^2]\]

The surface area of one finned row is the product of the specific surface of the finned tubes, the length of the finned tubes and the number of tubes in a row. The surface area of the fin bank was calculated with equation EV.8.
The pressure drop of the fluid was calculated with equation EV.21:

$$\Delta \rho = \frac{0.00517 \cdot f \cdot v^2 \cdot \rho \cdot L_{\text{hydr}}}{D_i}$$

where
- $\Delta \rho$ = pressure drop [psi]
- $f$ = Fanning friction factor [-]
- $\rho$ = density of the fluid [lb/ft$^3$]
- $L_{\text{hydr}}$ = total hydraulic length of the heater [ft]

The total hydraulic length is the length of the tubes plus 50 times the inner diameter of the tubes for every u-turn.

Example calculation of the fired heater

The exit temperature of the fired heater equals the reactor inlet temperature. This temperature should be 742.7 °F. The inlet temperature of the fired heater equals the outlet temperature of the heat exchanger H15. This temperature is 361.1 °F.

The total amount of heat adsorbed is 36.9 MBtu/h. This was calculated by ChemCad III.

The efficiency was calculated with equation EV.2. Figure 3, Berman (1978) shows the heat available as a function of the temperature and the percentage excess air for a refinery gas with a LHV of 19,700 Btu/lb. The LHV of the refinery gas used here is 24,700 Btu/lb so this Figure could not be used. The difference between the LHV and the heat available at a certain temperature is the heat needed to heat the flue gas to that temperature. So the curve is a function of the flue gas composition obtained by the combustion of the refinery gas. It was assumed that the composition of the flue gas in this process is the same as the composition of the flue gas of Figure 3, Berman (1978), so the slope of this Figure is the same as the slope of the Figure which shows the heat available as a function of the temperature for a gas with LHV of 24,700 Btu/lb. This resulted in an efficiency of 87.9 %.

In the radiant section tubes were selected with an outer diameter of 4.5 inch and an inner diameter of 4.0 inch. The fluid velocity was calculated with equation EV.3 and should be between 30 and 90 ft/s. Twenty passes were selected, to keep the pressure drop low, so the fluid velocity through the tubes is 62.6 ft/s.

The radiant heat duty calculated with equation EV.4 is 26.6 MBtu/h, so the convection heat duty is 10.3 MBtu/h.

In the radiant section an average radiant rate of 10,000 Btu/h/ft$^2$ was assumed, so the surface area needed in the radiant section is 2663 ft$^2$.

The diameter of the circle of the radiant tubes is 12.7 ft, so the length of the shield bank rows is 11 ft. A shield row consists of tubes with a centre to centre distance of 8 inch. Since the maximum width is 11 ft only 16 tubes fit in a row. Since there are 20 passes 10 tubes were selected in a row and the other 10 rows were placed on top of the first 10 tubes with a triangular pitch of 8 inch. All twenty tubes were considered to be in one row. The surface area of one shield row is 259 ft$^2$, so the surface area of the tubes in the radiant section is 2404 ft$^2$. This can be achieved with radiant tubes with a length of 34 ft.
The temperature of the flue gas above the shield bank was assumed to be 1260 °F.

The overall heat transfer coefficient in the shield bank was calculated by equation EV.9. The resistances $R_m, R_a$, and $R_i$ were first calculated. These values are respectively $0.154; 0.0008$ and $0.161$ h.ft$^2$°F/Btu, so the overall heat transfer coefficient, $U$, is 6.2 Btu/h/ft$^2$/°F.

Since the shield bank was considered to consist of three rows the total surface area of the shield bank is 777 ft$^2$.

A temperature increase of the fluid over the shield bank of 10°F was assumed. The log mean temperature difference over the shield bank is 857 °F.

The heat duty of the shield bank was calculated with equation EV.8. This heat duty is 4.1 MBtu/h. Equation EV.17 then gives the heat available at the shield bank. Out of the adapted Figure 3 of Berman the corresponding temperature of the flue gas above the shield bank was found. This is 1260 °F, as assumed.

The heat duty of the fin bank, calculated with equation EV.18, was 6.2 MBtu/h.

It was assumed that the tubes in the fin bank have 3 fins per inch, with a height of the fins of 0.75 in and a thickness of 0.05 in. This resulted in a total surface area of the finned tubes of 7.4 ft$^2$/ft and a fin efficiency of 84%. The surface area of one fined row is 1620 ft$^2$.

The overall heat transfer coefficient for this section is 2.2 Btu/h/ft$^2$/°F. Equation EV.8 then leads to a total needed surface area of 7487 ft$^2$, so 4.6 finned convection rows are needed. Since only an integer number of rows can be installed, 5 finned convection rows were selected.

The pressure drop over the fired heater was calculated with equation EV.21.

The hydraulic length of the shield bank plus the convection bank is 8 times the length of a convection tube plus a compensation for 7 u-turns. This is 205 ft.

The hydraulic length of the radiant bank is 3 times the length of a radiant tube plus a compensation for 2 u-turns. This equals 135 ft.

To compensate for the flow from the shield bank to the radiant section, and at the inlet and outlet of the fired heater 50 ft is added to the hydraulic length. So the total hydraulic length of the fired heater is 390 ft.

The Reynolds number is 770,000, so in Figure 12.24, Sinnott (1992), the Fanning friction factor was found to be 0.0017. This resulted in a pressure drop of 7.2 psi.
**EVI Design of a gas/liquid separator**

The gas/liquid separators were designed according to the method described by Olujic (1994). A difference has to be made between a horizontal and a vertical gas/liquid separator. A vertical position is preferred except in the case of large liquid to gas flow ratios. Here the design method for the vertical gas/liquid separator, V29, is given.

The diameter of the gas/liquid separator was calculated with equation EVI.1:

\[ d = 1.1284 \cdot \frac{M_g}{\rho_g \cdot u} \]  

where:
- \( d \) = diameter of the separator [m]
- \( M_g \) = mass flow of gas [kg/s]
- \( \rho_g \) = gas density [kg/m³]
- \( u \) = allowable gas velocity [m/s]

The allowable gas velocity is given by the empirical Sounders-Brown relation, equation EVI.2:

\[ u = C_{\text{drum}} \cdot \sqrt{\frac{\rho_l - \rho_g}{\rho_g}} \]  

where:
- \( C_{\text{drum}} \) = capacity coefficient [m/s]
- \( \rho_l \) = liquid density [kg/m³]

The capacity coefficient can be determined in several ways. Here the method from Olujic (1994) was used. In this method the capacity coefficient can be read from Figure 6.6, Olujic (1994).

The height of the separator was calculated with equation EVI.3:

\[ h = h_l + h_{lg} + h_{fg} \]  

where:
- \( h \) = height of the separator [m]
- \( h_l \) = height of the liquid level [m]
- \( h_{lg} \) = distance between maximum liquid level and feed inlet [m]
- \( h_{fg} \) = height of the separator above the feed inlet [m]

The height of the liquid level in the separator was calculated with equation EVI.4:

\[ h_l = \frac{4 \cdot V_l}{\pi \cdot d^2} \]  

where:
- \( V_l \) = volume of liquid [m³]
The volume of liquid in the separator is the product of the volumetric liquid flow and the hold-up time. A typical value of the hold-up time for a gas/liquid separator is 10 minutes, but for a gas/liquid separator upstream a compressor this should be 20 minutes. For the distance between the maximum liquid level and the feed inlet a value of 0.5 m was chosen. The height above the feed inlet is normally set at 1 time the diameter of the separator.

To prevent liquid droplets from being entrained in the gas stream, flowing to the compressor, a demister was installed.
Calculation of the gas/liquid separator V29

The gas- and liquid densities and the gas- and liquid flows were calculated by the process simulation program ChemCadIII. These values are summarized in Table EVI.1.

<table>
<thead>
<tr>
<th>Table EVI.1 - Gas- and liquid densities and flows</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas density [kg/m$^3$]</td>
</tr>
<tr>
<td>Liquid density [kg/m$^3$]</td>
</tr>
<tr>
<td>Gas flow [kg/s]</td>
</tr>
<tr>
<td>Liquid flow [kg/s]</td>
</tr>
</tbody>
</table>

With these values the dimensions of the gas/liquid separator were calculated.

Figure 6.6, Olujic (1994) gives $C_{down} = 0.11$ m/s. This results in a gas velocity of 1.8 m/s.

The diameter of the gas/liquid separator, as calculated by equation EVI.1 is 1.7 m. Since V29 is upstream compressor C19, the residence time of the liquid in the separator is 20 minutes. The height of the liquid level, calculated by EVI.4, is 3.4 m. The total height is 5.6 m.
EVII Design of a reflux drum for a distillation column

All the distillation columns were supported with a reflux drum to smoothen fluctuations in column operation and process upsets. This appendix describes the design of the reflux drum for column 1. The design is based on the method as described by Mehra (1979) and Younger (1955). In general horizontal drums are used.

In a reflux drum three different liquid levels can be given; the low liquid level (lll), the normal liquid level (nll) and the high liquid level (hll). The surge time between the nll and the lll should be about 5 minutes. If the volume stream out of the condenser of the column is known the surge volume is fixed.

\[ V_{\text{surge}} = t_{\text{surge}} \cdot \phi_v \]  

Where
- \( V_{\text{surge}} \) = surge volume [m³]
- \( t_{\text{surge}} \) = surge time [s]
- \( \phi_v \) = volume stream out of the condenser [m³/s]

According to Mehra the lll and the hll should both be 0.23 m. The nll should be at 50% of the diameter of the drum.

The economic optimum for the length/diameter ratio, given by Younger is 4. This results in the following equations:

\[ l = 4 \cdot D \]  

\[ V_{\text{surge}} = (1 - 2f) \cdot \frac{1}{2} \cdot \frac{\pi}{4} \cdot D^2 \cdot l \]  

where
- \( l \) = length of the drum [m]
- \( D \) = diameter of the drum [m]
- \( f \) = fraction of the volume of the drum from level nll till the lll [-]

The fraction \( f \) is a function of the diameter of the drum.

Calculation of the dimensions of the reflux drum for column 1

The volume stream out of the condenser of column 1 is 0.064 m/s, so the surge volume, calculated by equation EVII.1, is 19.2 m³. Equation EVII.2 and EVII.3 result in a diameter of the drum of 2.4 m and a length of 9.5 m. The fraction of the volume of the drum from the bottom till the lll is 0.11.
Appendix F

Process safety
**FI HAZOP analysis**

The results of the HAZOP-analysis are displayed in the following Tables. The numbers behind the actions required correspond with the numbers of the possible causes.

<table>
<thead>
<tr>
<th>Deviation</th>
<th>Possible causes</th>
<th>Consequences</th>
<th>Action required</th>
</tr>
</thead>
<tbody>
<tr>
<td>No feed flow</td>
<td>1. No feed</td>
<td>- No bottom and top products</td>
<td>- Good communication with supplier (1)</td>
</tr>
<tr>
<td></td>
<td>2. Line fracture</td>
<td>- Downstream units down</td>
<td>- Good maintenance of pipes and pumps (2-4)</td>
</tr>
<tr>
<td></td>
<td>3. Line blockage</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>4. Pump out of order</td>
<td></td>
<td></td>
</tr>
<tr>
<td>No bottom flow</td>
<td>1. No feed</td>
<td>- No bottom product</td>
<td>- Good communication with supplier (1)</td>
</tr>
<tr>
<td></td>
<td>2. Line fracture</td>
<td>- Temperature increase in column</td>
<td>- Good maintenance of pipes and pumps (2-4)</td>
</tr>
<tr>
<td></td>
<td>3. Line blockage</td>
<td>- Composition top stream changes</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4. Pump out of order</td>
<td></td>
<td></td>
</tr>
<tr>
<td>No distillate flow</td>
<td>1. No feed</td>
<td>- No top product</td>
<td>- Good communication with supplier (1)</td>
</tr>
<tr>
<td></td>
<td>2. Line fracture</td>
<td>- Reflux ratio changes</td>
<td>- Good maintenance of pipes and pumps (2-4)</td>
</tr>
<tr>
<td></td>
<td>3. Line blockage</td>
<td>- Composition bottom stream changes</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4. Pump out of order</td>
<td>- Downstream units down</td>
<td></td>
</tr>
<tr>
<td></td>
<td>5. Reflux drum empty</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6. Temperature in column to low</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7. No steam</td>
<td></td>
<td></td>
</tr>
<tr>
<td>No steam flow</td>
<td>1. No steam</td>
<td>- No vaporization</td>
<td>- Good communication with supplier (1)</td>
</tr>
<tr>
<td></td>
<td>2. Line fracture</td>
<td>- Column temperature decreases</td>
<td>- Good maintenance of pipes and pumps (2-3)</td>
</tr>
<tr>
<td></td>
<td>3. Line blockage</td>
<td>- Composition bottom and top products change</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Less top flow, more bottom flow</td>
<td></td>
</tr>
<tr>
<td>No air flow</td>
<td>1. No fan power</td>
<td>- No condensation</td>
<td>- Secondary power supply</td>
</tr>
<tr>
<td></td>
<td>2. Broken fan</td>
<td>- Column temperature increases</td>
<td>- Good maintenance (2)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Composition bottom and top products change</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>- More top flow, less bottom flow</td>
<td></td>
</tr>
<tr>
<td>Table F.2</td>
<td>Hazard and operability study for the reactor</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>---------------------------------------------</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
| **No feed flow** | **1. No feed**  
2. Line fracture  
3. Line blockage  
4. Pump out of order | **- No product (unit down)**  
- Downstream units down  
- Good communication with supplier (1)  
- Good maintenance of pipes and pumps (2-4) |
| **More flow** | **1. More feed**  
2. Line fracture - Downstream units down with supplier (1)  
3. Line blockage - Good maintenance of pipes and pumps (2-4) | **- Different reactor effluent composition**  
- Storage tank to compensate for fluctuations |
| **More pressure** | **1. Reactor feed at higher pressure** | **- Different reactor effluent composition**  
- Possible temperature increase due to more hydrogenation  
- PC at reactor outlet  
- TC at fired heater outlet |
| **More pressure drop** | **1. Attrition of catalyst particles** | **- Lower outlet pressure**  
- Timely replacement of catalyst |
| **More temperature** | **1. Heat duty of fired heater to high** | **- Different reactor effluent composition**  
- TC at fired heater outlet |
| **Less flow** | **1. Less feed**  
2. Line fracture - Downstream units down with supplier (1)  
3. Line blockage - Good maintenance of pipes and pumps (2-4) | **- Different reactor effluent composition**  
- Storage tank to compensate for fluctuations |
| **Less pressure** | **1. Compressor out of order**  
2. Pump out of order  
3. Lower feed temperature  
4. Leakage in pipeline  
5. Partly blocked pipeline | **- Different reactor effluent composition**  
- Good maintenance (1,2,4,5)  
- TC at fired heater outlet |
| **Less temperature** | **1. Heat duty of fired heater to low** | **- Different reactor effluent composition**  
- TC on fired heater outlet |
| **Products as well as impurities** | **1. Undesired reactions** | **- Impurities in products**  
- Clay-treatment |
| **Part of conversion** | **1. H₂/C₄ ratio deviation**  
2. Lower residence time  
3. Reactor pressure and temperature deviation | **- Different reactor effluent composition**  
- Recycle larger  
- CC on reactor inlet stream (1)  
- Storage tank to compensate for fluctuations (2)  
- TC on fired heater outlet and PC on reactor outlet(3) |
Table FI.3 Hazard and operability study for the gas/liquid separator

<table>
<thead>
<tr>
<th></th>
<th>1. No feed</th>
<th>- No gas and liquid flow</th>
<th>- Good maintenance (1-3)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No feed flow</td>
<td>2. Line fracture</td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3. Line blockage</td>
<td></td>
<td></td>
</tr>
<tr>
<td>More flow</td>
<td>1. More feed</td>
<td>- Higher liquid level</td>
<td>- LC on separator</td>
</tr>
<tr>
<td></td>
<td></td>
<td>- Higher pressure</td>
<td></td>
</tr>
<tr>
<td>More pressure</td>
<td>1. Higher inlet pressure</td>
<td>- Different composition and quantity gas and liquid flow</td>
<td>- PC on gas purge</td>
</tr>
<tr>
<td>More temperature</td>
<td>1. Cooler duty too low</td>
<td>- Different composition and quantity gas and liquid flow</td>
<td>- Good maintenance of cooler - TC in cooler outlet stream</td>
</tr>
<tr>
<td>Less flow</td>
<td>1. Less feed</td>
<td>- Lower liquid level</td>
<td>- LC on separator</td>
</tr>
<tr>
<td>Less pressure</td>
<td>1. Lower inlet pressure</td>
<td>- Different composition and quantity gas and liquid flow</td>
<td>- PC on gas purge</td>
</tr>
<tr>
<td>Less temperature</td>
<td>1. Cooler duty too high</td>
<td>- Different composition and quantity gas and liquid flow</td>
<td>- Good maintenance of the cooler - TC in cooler outlet stream</td>
</tr>
<tr>
<td>Liquid as well as gas in H2</td>
<td>1. Demister broken</td>
<td>- Liquid droplets in compressor : possible breakdown</td>
<td>- Good maintenance (1) - Storage drum before compressor</td>
</tr>
</tbody>
</table>
### Table FI.4 Hazard and operability study for the heat-exchangers and fired heater

<table>
<thead>
<tr>
<th>Heat-exchangers</th>
<th>1. No cooling or heating medium flow</th>
<th>- Temperature not on specified level L/V-ratio not at specified value</th>
<th>- Good maintenance (1,2) - Switch to other medium if possible (1) - TC in exchanger outlet stream</th>
</tr>
</thead>
<tbody>
<tr>
<td>No Cooling/Heating</td>
<td>2. Heat-exchanger broken</td>
<td>- Good maintenance (l,2)</td>
<td></td>
</tr>
<tr>
<td>Fired heater</td>
<td>1. No fuel</td>
<td>- No temperature increase of process fluid</td>
<td>- Good communication with supplier (1) - Good maintenance (2,3)</td>
</tr>
<tr>
<td>No fuel flow</td>
<td>2. Line fracture</td>
<td>- Good communication with supplier (1) - Good maintenance (2,3)</td>
<td></td>
</tr>
<tr>
<td>No air flow</td>
<td>3. Line blockage</td>
<td>- No temperature increase of process fluid</td>
<td>- Secondary power supply (1) - Good maintenance (2-4)</td>
</tr>
<tr>
<td>No feed flow</td>
<td>1. No feed</td>
<td>- Overheating of tubes</td>
<td>- Low flow alert on fired heater feed (1-4) - Good maintenance (2-4)</td>
</tr>
<tr>
<td>More fuel flow</td>
<td>2. Line fracture</td>
<td>- Temperature increase</td>
<td>- TC in process outlet stream - FC in fuel stream</td>
</tr>
<tr>
<td>More air flow</td>
<td>3. Line blockage</td>
<td>- Temperature decrease</td>
<td>- TC in process outlet stream - FFC in fuel and air streams</td>
</tr>
<tr>
<td>Less fuel flow</td>
<td>4. Pump and compressor out of order</td>
<td>- Good communication - Fuel storage - TC in process outlet stream - FC on fuel stream</td>
<td></td>
</tr>
<tr>
<td>Less air flow</td>
<td>1. Less fuel</td>
<td>- Temperature decrease</td>
<td>- Good maintenance fan - TC in process outlet stream - FFC in fuel and air stream</td>
</tr>
<tr>
<td>Less air flow</td>
<td>- First temperature increase, then temperature decrease</td>
<td>- Good maintenance fan - TC in process outlet stream - FFC in fuel and air stream</td>
<td></td>
</tr>
</tbody>
</table>

### Table FI.5 Hazard and operability study for the pump and the compressor

<table>
<thead>
<tr>
<th>Reverse flow</th>
<th>1. Pump or compressor failure</th>
<th>- Reverse flow</th>
<th>- No-return valve in outlet stream - Good maintenance</th>
</tr>
</thead>
</table>

F - 4
### FII. Dow fire and explosion index calculation

**Table FII.2** MAC-value, NFPA classification, material factor and explosion limits

<table>
<thead>
<tr>
<th>Component</th>
<th>MAC-value structure formula</th>
<th>MAC-value</th>
<th>NFPA classification</th>
<th>Material factor</th>
<th>Explosion limits (vol% in air)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component</td>
<td>(ppm)</td>
<td>(mg/m³)</td>
<td>N_H</td>
<td>N_F</td>
<td>N_R</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>n.d.</td>
<td>0</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Methane</td>
<td>CH₄</td>
<td>n.d.</td>
<td>1</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Ethane</td>
<td>C₂H₆</td>
<td>n.d.</td>
<td>1</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Propane</td>
<td>C₃H₈</td>
<td>n.d.</td>
<td>1</td>
<td>4</td>
<td>0</td>
</tr>
<tr>
<td>Benzene</td>
<td>C₆H₆</td>
<td>10 30</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>Toluene</td>
<td>C₇H₈</td>
<td>40 140</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>C₈H₁₀</td>
<td>50 215</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>para-Xylene¹</td>
<td>C₈H₁₀</td>
<td>n.d.</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>meta-Xylene¹</td>
<td>C₈H₁₀</td>
<td>100 435</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>ortho-Xylene¹</td>
<td>C₈H₁₀</td>
<td>n.d.</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>Cumene</td>
<td>C₉H₁₀</td>
<td>25 120</td>
<td>2</td>
<td>3</td>
<td>0</td>
</tr>
<tr>
<td>1,2,4-trimethylbenzene</td>
<td>C₁₀H₁₂</td>
<td>25 125</td>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>para-Diethylbenzene</td>
<td>C₁₀H₁₄</td>
<td>n.d.</td>
<td>2</td>
<td>2</td>
<td>0</td>
</tr>
</tbody>
</table>

¹ Data for xylene are taken.
² n.d. = not determined

**Table FII.2** Corrected N_F and material factors

<table>
<thead>
<tr>
<th>Component</th>
<th>N_F</th>
<th>Material factor</th>
<th>Component</th>
<th>N_F</th>
<th>Material factor</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>4</td>
<td>21</td>
<td>para-Xylene¹</td>
<td>4</td>
<td>21</td>
</tr>
<tr>
<td>Methane</td>
<td>4</td>
<td>21</td>
<td>meta-Xylene¹</td>
<td>4</td>
<td>21</td>
</tr>
<tr>
<td>Ethane</td>
<td>4</td>
<td>21</td>
<td>ortho-Xylene¹</td>
<td>4</td>
<td>21</td>
</tr>
<tr>
<td>Propane</td>
<td>4</td>
<td>21</td>
<td>Cumene</td>
<td>4</td>
<td>21</td>
</tr>
<tr>
<td>Benzene</td>
<td>4</td>
<td>21</td>
<td>1,2,4-trimethylbenzene</td>
<td>3</td>
<td>16</td>
</tr>
<tr>
<td>Toluene</td>
<td>4</td>
<td>21</td>
<td>para-Diethylbenzene</td>
<td>3</td>
<td>16</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>4</td>
<td>21</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
General process hazards factor

The following penalties were assigned to the gas-recycle:

<table>
<thead>
<tr>
<th>Description</th>
<th>Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base factor</td>
<td>1.00</td>
</tr>
<tr>
<td>Mild exothermic reaction</td>
<td>0.30</td>
</tr>
<tr>
<td>Presence of N_H = 3 or 4 flammable liquids or gases</td>
<td>0.85</td>
</tr>
<tr>
<td>Drainage and spill control</td>
<td>0.50</td>
</tr>
<tr>
<td><strong>General process hazards factor</strong></td>
<td>2.65</td>
</tr>
</tbody>
</table>

The assumption was made that the area housing the unit was well accessible (at least from two sides, with one side being a road). Therefore no penalty was taken into account for this item.

The penalty for drainage and spill control was taken to be the maximum possible. If more data were available, the penalty could further be specified.

Special process hazards factor

The following penalties were assigned to the gas-recycle:

<table>
<thead>
<tr>
<th>Description</th>
<th>Penalty</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base factor</td>
<td>1.00</td>
</tr>
<tr>
<td>Toxic materials present</td>
<td>0.40</td>
</tr>
<tr>
<td>Ability for air to enter the system</td>
<td>0.50</td>
</tr>
<tr>
<td>High pressure of compressed gases</td>
<td>0.36</td>
</tr>
<tr>
<td>Quantity of flammable materials</td>
<td>1.00</td>
</tr>
<tr>
<td>Average penalty for corrosion</td>
<td>0.35</td>
</tr>
<tr>
<td>Leakage</td>
<td>0.10</td>
</tr>
<tr>
<td>Use of fired heater</td>
<td>0.25</td>
</tr>
<tr>
<td><strong>Special process hazards factor</strong></td>
<td>3.96</td>
</tr>
</tbody>
</table>

The penalty for the ability of air entering the system and the penalty for the pressurized gases were estimated by assuming the worst possible situations.

The quantity of flammable material was determined by taking the massflow of the largest stream present in the unit. In the stream which originates from the reactor the total flow was 66,201 kg/h. Combining this with the enthalpy of combustion for the different components present gave a total energy release of 4.77*10^8 Btu. From Figure 3, Dow F&EI (1987) it followed that the penalty should be 1.00.

For corrosion of the construction material an average penalty was taken, because no data about the corrosion rates were found.

The penalty for leakage of gaskets, seals of joints or shafts and packing was determined by assuming that only minor leakage occurred.
The penalty taken into account for the use of a fired heater in the gas recycle was estimated by assuming that the distance between the fired heater and a possible leak source is 105 feet. From Figure 6, Dow F&EI (1987), taking the A-2 curve (for materials raised above their boiling point), a penalty of 0.25 was taken into account.
Appendix G

Component properties
Appendix G: Component properties

Table G.1 shows the material properties of the components used in the process. The literature used for this Table is the Lide (1995), Reid (1987), Lewis (1992) and the 'Chemiekaarten' (1996). The prices were provided by Raytheon.

Table G.1: Component properties of the compounds being present in the process.

<table>
<thead>
<tr>
<th>Component</th>
<th>Hydrogen</th>
<th>Methane</th>
<th>Ethane</th>
<th>Propane</th>
<th>Benzene</th>
<th>Toluene</th>
<th>EB</th>
</tr>
</thead>
<tbody>
<tr>
<td>Formula</td>
<td>H2</td>
<td>CH4</td>
<td>C2H6</td>
<td>C3H8</td>
<td>C6H6</td>
<td>C6H6</td>
<td>C8H10</td>
</tr>
<tr>
<td>Molecular weight [g/mol]</td>
<td>2.016</td>
<td>16.04</td>
<td>30.07</td>
<td>44.1</td>
<td>78.11</td>
<td>92.14</td>
<td>106.17</td>
</tr>
<tr>
<td>Boilingpoint [°C]</td>
<td>-252.85</td>
<td>-161.55</td>
<td>-88.55</td>
<td>-42.05</td>
<td>80.05</td>
<td>110.65</td>
<td>136.15</td>
</tr>
<tr>
<td>Meltingpoint [°C]</td>
<td>-259.15</td>
<td>-182.45</td>
<td>-183.25</td>
<td>-187.65</td>
<td>5.55</td>
<td>-95.15</td>
<td>-94.95</td>
</tr>
<tr>
<td>Liquid density 20°C [kg/m³]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>0.8765</td>
<td>0.8669</td>
<td>0.867</td>
</tr>
<tr>
<td>MAC-value [ppm - mg/m³]</td>
<td>not det.</td>
<td>not det.</td>
<td>not det.</td>
<td>not det.</td>
<td>10</td>
<td>40</td>
<td>50</td>
</tr>
<tr>
<td>Price [US$/ton]</td>
<td>1000</td>
<td>C7 stream: 150</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Explosion limits in air [vol%]</td>
<td>4.0 - 76</td>
<td>4.4 - 16</td>
<td>2.7 - 12.5</td>
<td>1.7 - 9.5</td>
<td>1.2 - 8.0</td>
<td>1.2 - 7</td>
<td>1.0 - 6.7</td>
</tr>
<tr>
<td>Heat of vaporization, T_{boil} [kJ/mol]</td>
<td>0.898</td>
<td>8.19</td>
<td>14.69</td>
<td>19.04</td>
<td>30.72</td>
<td>33.18</td>
<td>35.57</td>
</tr>
<tr>
<td>Heat of vaporization, 25°C [kJ/mol]</td>
<td>-</td>
<td>-</td>
<td>5.16</td>
<td>14.79</td>
<td>33.83</td>
<td>38.01</td>
<td>42.24</td>
</tr>
<tr>
<td>Cp = A + B<em>T + C</em>T² + D*T² [J/mol·K]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A /10³</td>
<td>2.714</td>
<td>1.925</td>
<td>0.541</td>
<td>-0.422</td>
<td>-3.392</td>
<td>-2.435</td>
<td>-4.310</td>
</tr>
<tr>
<td>B /10³</td>
<td>0.093</td>
<td>0.521</td>
<td>1.781</td>
<td>3.063</td>
<td>4.739</td>
<td>5.125</td>
<td>7.072</td>
</tr>
<tr>
<td>C /10⁴</td>
<td>-0.138</td>
<td>0.120</td>
<td>-0.694</td>
<td>1.586</td>
<td>-3.017</td>
<td>-2.765</td>
<td>-4.811</td>
</tr>
<tr>
<td>D /10⁸</td>
<td>0.765</td>
<td>-1.132</td>
<td>0.871</td>
<td>3.215</td>
<td>7.130</td>
<td>4.911</td>
<td>13.010</td>
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<tr>
<td>Enthalpy of formation /10⁶ [J/mol]</td>
<td>0.000</td>
<td>-7.490</td>
<td>-8.474</td>
<td>-10.390</td>
<td>8.298</td>
<td>5.003</td>
<td>2.981</td>
</tr>
<tr>
<td>Component</td>
<td>p-Xylene</td>
<td>m-Xylene</td>
<td>o-Xylene</td>
<td>Cumene</td>
<td>1,2,4-TMB</td>
<td>p-DEB</td>
<td></td>
</tr>
<tr>
<td>---------------</td>
<td>----------</td>
<td>----------</td>
<td>----------</td>
<td>--------</td>
<td>-----------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>Formula</td>
<td>C₈H₁₀</td>
<td>C₈H₁₀</td>
<td>C₈H₁₀</td>
<td>C₉H₁₂</td>
<td>C₁₀H₁₂</td>
<td>C₁₀H₁₄</td>
<td></td>
</tr>
<tr>
<td>Molecular weight</td>
<td>[g/mol]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>106.17</td>
<td>106.17</td>
<td>106.17</td>
<td>120.19</td>
<td>120.19</td>
<td>134.22</td>
<td></td>
</tr>
<tr>
<td>Boilingpoint</td>
<td>[°C]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>138.35</td>
<td>139.15</td>
<td>144.45</td>
<td>152.45</td>
<td>169.35</td>
<td>183.75</td>
<td></td>
</tr>
<tr>
<td>Meltingpoint</td>
<td>[°C]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>13.45</td>
<td>-47.85</td>
<td>-25.15</td>
<td>-96.05</td>
<td>-46.15</td>
<td>-42.15</td>
<td></td>
</tr>
<tr>
<td>Liquid density 20°C</td>
<td>[kg/m³]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>0.8611</td>
<td>0.8642</td>
<td>0.8802</td>
<td>0.8618</td>
<td>0.8758</td>
<td>0.8602</td>
<td></td>
</tr>
<tr>
<td>MAC-value</td>
<td>[ppm - mg/m³]</td>
<td>not det.</td>
<td>not det.</td>
<td>25</td>
<td>25</td>
<td>not det.</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>100</td>
<td>435</td>
<td></td>
<td></td>
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</tr>
<tr>
<td>Price</td>
<td>[US$/ton]</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>400</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Explosion limits in air</td>
<td>[vol%]</td>
<td>1.1 - 7.0</td>
<td>1.1 - 7.0</td>
<td>1.0 - 7.6</td>
<td>0.8 - 6.0</td>
<td>0.9 - 6.4</td>
<td>0.8 - 5</td>
</tr>
<tr>
<td>Heat of vaporization, T_{boil}</td>
<td>[kJ/mol]</td>
<td>35.67</td>
<td>35.66</td>
<td>36.24</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Heat of vaporization, 25°C</td>
<td>[kJ/mol]</td>
<td>42.4</td>
<td>42.62</td>
<td>43.43</td>
<td>45.13</td>
<td>47.93</td>
<td></td>
</tr>
<tr>
<td>Enthalpy of formation /10⁴ [J/mol]</td>
<td></td>
<td>1.796</td>
<td>1.725</td>
<td>1.900</td>
<td>0.394</td>
<td>-1.394</td>
<td>-2.227</td>
</tr>
</tbody>
</table>
Appendix H

Economics
H. Economics

H.1 Calculation of costs

The total costs can be calculated with the following equation:

\[ K_T = 1.13 \cdot K_p + 2.6 \cdot L + (0.13 + c) \cdot I_T \]

where:
- \( K_T \) = total costs [\$/year]
- \( K_p \) = production volume related costs [\$/year]
- \( L \) = operating labour related costs [\$/year]
- \( c \) = capital charge [-]
- \( I_T \) = total investment costs [\$/year]

The capital charge is read from Table IV-9, Montfoort (1991): \( c = 0.149 \)

The production volume related costs, the operating labour related costs and the total investment costs were calculated as shown below. This resulted in a total costs; \( K_T \) = 47.7 M$/year

Production volume related costs

To obtain the production volume related costs, the price and quantity of the mixed xylenes stream and hydrogen stream as well as the quantities and prices of all used utilities were needed. The production volume related costs are calculated in Table H.1.

Table H.1 Calculation of production volume related costs

<table>
<thead>
<tr>
<th>Stream</th>
<th>kton/year</th>
<th>k$/kton</th>
<th>k$/year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed xylenes</td>
<td>130.0</td>
<td>150</td>
<td>19,500</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1.46</td>
<td>1000</td>
<td>1,464</td>
</tr>
<tr>
<td>MP steam</td>
<td>340.7</td>
<td>19.1</td>
<td>6,507</td>
</tr>
<tr>
<td>Cooling water</td>
<td>11,030.3</td>
<td>0.06</td>
<td>650.8</td>
</tr>
<tr>
<td>Fuel gas</td>
<td>354,826</td>
<td>4.83</td>
<td>1,714</td>
</tr>
<tr>
<td>Electricity</td>
<td>2,869</td>
<td>76.47</td>
<td>219.4</td>
</tr>
<tr>
<td>Catalyst</td>
<td>12.31</td>
<td>29.4</td>
<td>362.1</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td>30,417</td>
</tr>
</tbody>
</table>
Operating labour related costs

The costs related to the operating labour were calculated with the Wessel equation, Montfoort (1991):

\[ L = 32 \cdot N \cdot P^{0.24} \]

where

- \( L \) = operating labour related costs [kfl/year]
- \( N \) = number of process steps [-]
- \( P \) = capacity of the process [kton/year]

There are five process steps, and the capacity is 103.5 kton/year.

\[ L = 487 \text{ kfl} = 287 \text{ M\$/year} \quad \text{(rate of exchange: \$1.00 = fl. 1.70)} \]

Total investment costs

The investment costs are the most important in determining if the process is profitable. The investment costs can be divided into four groups:

\[ I_T = I_B + I_H + I_L + I_W \]

where

- \( I_T \) = total investment costs [\$]
- \( I_B \) = investments in process units (64% of total) [\$]
- \( I_H \) = investments in auxiliary facilities (16% of total) [\$]
- \( I_L \) = investments in miscellaneous capital (14% of total) [\$]
- \( I_W \) = investments in working capital (6% of total) [\$]

The sum of \( I_B \) and \( I_H \) are the fixed capital costs. The total investment costs were estimated by calculating the investments in process units (\( I_B \)). These costs are 64% of the total costs. The total costs were calculated by multiplying \( I_B \) by 100/64. \( I_B \) can be calculated with various methods. The methods of Zevnik-Buchanan, Wilson and Taylor were used.

Method of Zevnik-Buchanan

The modified Zevnik-Buchanan-Jansen method was used. This method assumes that the investments depend on the process capacity and the process complexity. For the calculation of the investment costs the following data were needed:

- process capacity
- number of functional units
- complexity factor
- plant cost index
The process was divided in seven functional units:

1. Distillation column T1
2. Distillation column T16
3. Distillation column T7
4. Reactor R23
5. p-Xylene separator V8
6. Clay-tower T14
7. Fired heater F20, L/V-separator V29

The complexity factor was calculated for every functional unit with the following equation:

\[ C_j = 2 \cdot 10^{(F_t \cdot F_p \cdot F_m)} \]  

where
- \( C_t \) = complexity factor
- \( F_t \) = temperature factor
- \( F_p \) = pressure factor
- \( F_m \) = material factor

The temperature factor is given by:

\[ F_t = 0.018 \cdot \left( \frac{T - 290}{100} \right) \]  

if \( T > 290 \), and

\[ F_t = -0.2 \cdot \left( \frac{T - 290}{100} \right) \]  

if \( T \leq 290 \)

where \( T \) = maximal possible temperature

The pressure factor and the material factor can be read from Figure III-17 and Table III-18 respectively, Montfoort (1991).

The total investment in process units were calculated with:

\[ I_g = 0.1 \cdot \left( \sum_{i=1}^{N} C_{ji} \cdot P_i^m \right) \cdot C_i \]  

where
- \( N \) = number of functional units
- \( P_i \) = capacity
- \( C_i \) = CE-Plant Cost Index

\[ I_g \] = cost of process units
The CE-Plant Cost Index was obtained from the Chemical Engineering journal and is for July 1996: 381.1.

For every unit the complexity factor was determined. With equation H.7 the total investment costs for the units were calculated. The total investment costs were obtained by multiplying by 100/64. The calculations are shown in Table H.2.

Table H.2 Calculation of total investment costs with method of Zevnik-Buchanan

<table>
<thead>
<tr>
<th>Unit</th>
<th>( F_t )</th>
<th>( F_p )</th>
<th>( F_m )</th>
<th>( C_r )</th>
<th>( P ) [kton/year]</th>
<th>( I_B ) [MS]</th>
<th>( I_T ) [MS]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Distillation T1</td>
<td>0.024</td>
<td>0.015</td>
<td>0</td>
<td>2.19</td>
<td>480.89</td>
<td>3.39</td>
<td>5.30</td>
</tr>
<tr>
<td>Distillation T16</td>
<td>0.027</td>
<td>0.015</td>
<td>0</td>
<td>2.20</td>
<td>34.55</td>
<td>0.70</td>
<td>1.10</td>
</tr>
<tr>
<td>Distillation T7</td>
<td>0.023</td>
<td>0.01</td>
<td>0</td>
<td>2.16</td>
<td>374.71</td>
<td>2.88</td>
<td>4.49</td>
</tr>
<tr>
<td>Reactor R23</td>
<td>0.070</td>
<td>0.09</td>
<td>0</td>
<td>2.89</td>
<td>529.63</td>
<td>4.75</td>
<td>7.42</td>
</tr>
<tr>
<td>para-Xylene separator</td>
<td>0.054</td>
<td>0.015</td>
<td>0</td>
<td>2.34</td>
<td>446.33</td>
<td>3.47</td>
<td>5.43</td>
</tr>
<tr>
<td>Clay-tower</td>
<td>0.023</td>
<td>0.03</td>
<td>0</td>
<td>2.26</td>
<td>350.89</td>
<td>2.90</td>
<td>4.52</td>
</tr>
<tr>
<td>Fired heater L/V-separator</td>
<td>0.068</td>
<td>0.09</td>
<td>0</td>
<td>2.88</td>
<td>529.63</td>
<td>4.73</td>
<td>7.39</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>22.82</td>
<td>35.66</td>
<td></td>
</tr>
</tbody>
</table>

**Method of Wilson**

This method uses all units except the pumps and compressors, the average capacity and the average costs of the units. From Figures III-26 and III-27, Montfoort (1991) the temperature factor, the pressure factor and the material factor were obtained. The average costs were calculated with:

\[
AUC = 21 \cdot (P_{av})^{0.675} \tag{H.8}
\]

where

- \( AUC \) = average costs per unit
- \( P_{av} \) = average capacity per unit [ton/year] [£]
The investments can be calculated with:

\[ I_B = f \cdot N \cdot AUC \cdot F_t \cdot F_p \cdot F_m \cdot \frac{C_t}{C_0} \]  

where:
- \( f \) = investment factor
- \( N \) = number of units (except pumps and compressors)
- \( C_t \) = PE-Plant Cost Index in july 1996
- \( C_0 \) = PE-Plant Cost Index, 115 in 1971

There are 18 equipments (except pumps and compressors).
The average capacity is: 426.33 kton/year.

With this capacity the average costs of an unit were determined with equation H.8:

\[ AUC = k \cdot 132.5 \]

The temperature factor, pressure factor and material factor are respectively: \( F_T = 1.08 \), \( F_p = 1 \), \( F_m = 1 \).

The investment factor was obtained from Figure III-28, Montfoort (1991) and is: \( f = 1.6 \)

The EP-Cost Index is:
- 1971: 115
- 1977: 300
- 1979: 363
- 1980: 100
- 1989: 135
- 1990: 100

So \( C_t \) in july 1996 is 623.3

With equation H.9 the total investments were finally calculated:
\[ I_B = 13.66 \text{ ME} = 20.49 \text{ M$} \text{ (rate of exchange £/S = 1.65)} \]
\[ I_T = 32.02 \text{ M$} \]

**Method of Taylor**

This method is based on the number of process steps and not on the number of units. The investment costs can be calculated with:

\[ I_B = 45 \cdot f \cdot p^{0.39} \cdot \frac{C_t}{C_0} \]  

where:
- \( f \) = costliness index
- \( C_t \) = PE-Plant Cost Index in july 1996
- \( C_0 \) = PE-Plant Cost Index, 300 in 1977
The costliness index can be calculated with:

\[ f = \sum_{i=1}^{N} (1.3)^{S_i} \]

where \( N \) = number of process steps
\( S_i \) = complexity score for a process step

The complexity scores for the process steps and calculation of the costliness index are shown in Table H.3.

### Table H.3  Complexity scores and costliness index calculations

<table>
<thead>
<tr>
<th>Streams</th>
<th>Capacity</th>
<th>Material</th>
<th>Reaction time</th>
<th>Pressure and temperature</th>
<th>Multi streaming</th>
<th>( S_i )</th>
<th>( 1.3^{S_i} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mixed xylenes (fresh)</td>
<td>0.37</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.37</td>
<td>1.10</td>
</tr>
<tr>
<td>Mixed xylenes (recycle)</td>
<td>2.2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2.2</td>
<td>1.78</td>
</tr>
<tr>
<td>( H_2 ) (fresh)</td>
<td>-5.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-5.0</td>
<td>0.27</td>
</tr>
<tr>
<td>( H_2 ) (recycle)</td>
<td>0.60</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0.60</td>
<td>1.17</td>
</tr>
<tr>
<td>Water</td>
<td>8.9</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>8.9</td>
<td>10.33</td>
</tr>
<tr>
<td>MD steam</td>
<td>3.1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.1</td>
<td>2.26</td>
</tr>
<tr>
<td>\textit{para-Xylene and ortho-Xylene} &amp; 0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>( C_8)'-stream</td>
<td>-7.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-7.0</td>
<td>0.16</td>
</tr>
<tr>
<td>( C_7)'-stream</td>
<td>-2.8</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-2.8</td>
<td>0.48</td>
</tr>
<tr>
<td>Fuel gas</td>
<td>-5.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-5.0</td>
<td>0.27</td>
</tr>
<tr>
<td>Processes</td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Distillation T1</td>
<td>2.8</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2.8</td>
<td>2.08</td>
</tr>
<tr>
<td>Distillation T16</td>
<td>-1.9</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-1.9</td>
<td>0.61</td>
</tr>
<tr>
<td>Distillation T7</td>
<td>2.3</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>2.3</td>
<td>1.83</td>
</tr>
<tr>
<td>Reaction R23</td>
<td>3.0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>3.0</td>
<td>2.20</td>
</tr>
<tr>
<td>\textit{para-Xylene separation} &amp; 2.7</td>
<td>0</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>4.7</td>
<td>3.43</td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>28.97</td>
</tr>
</tbody>
</table>
With equation H.10 the total investment costs were calculated:
\[ I_B = 16.54 \text{ M€} = 27.30 \text{ MS} \]
\[ I_T = 42.65 \text{ MS} \]

For the total investment costs the average value of the three different methods was used:
\[ I_T = 45.30 \text{ MS}. \]

**H.2 Calculation of the income**

The total income was calculated and is presented in Table H.4.

<table>
<thead>
<tr>
<th>Stream</th>
<th>kton/year</th>
<th>k$/kton</th>
<th>MS/year</th>
</tr>
</thead>
<tbody>
<tr>
<td>para-Xylene</td>
<td>71.15</td>
<td>500</td>
<td>35.58</td>
</tr>
<tr>
<td>ortho-Xylene</td>
<td>32.36</td>
<td>400</td>
<td>12.94</td>
</tr>
<tr>
<td>C7-stream</td>
<td>23.82</td>
<td>150</td>
<td>3.57</td>
</tr>
<tr>
<td>C9+ -stream</td>
<td>2.20</td>
<td>200</td>
<td>0.44</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td></td>
<td><strong>52.53</strong></td>
</tr>
</tbody>
</table>

The annual profit before taxes is: total income - total production costs. This equals 4.8 MS/year.

**H.3 Economical criteria**

**Return On Investment**

This criterium gives the percentage of the investments which is returned annually. To obtain this percentage the annual profit should be divided by the investment costs in fixed capital and working capital:

\[
ROI = \left( \frac{W}{I_F + I_W} \right) \times 100\% 
\]  

where  
\[ W = \text{annual profit before taxes} \]  
\[ I_F = \text{investment costs in fixed capital} \]  
\[ I_W = \text{investment costs in working capital} \]  

For a plant life of 10 years the ROI should at least be 10%.
With equation H.12 the ROI was calculated:

\[ \text{ROI} = 12.4\% \]

**Pay-Out-Time**

Another measure to assess profitability is the Pay-Out-Time, which is the time to recover the fixed capital investments. The Pay-Out-Time is calculated with the following equation:

\[ \text{POT} = \frac{l_p}{V - (K_p + 2.6 \cdot L)} \]  

where  
\[ V = \text{total income} \]  
\[ [\text{S/year}] \]

The Pay-Out-Time for this process is:

\[ \text{POT} = 1.7 \text{ years} = 20 \text{ months} \]

**Internal Rate of Return**

The Internal Rate of Return criterion also gives the percentage of investments which is returned annually. But this method also accounts for the change in value of money over the years. With this method the cash flows, during the life time of the plant, are converted to the present value with such a return percentage that the sum of these discounted cash flows over the plant life time is zero. This method assumes that the incoming cash flows during the plant life are directly reinvested in other projects with the same return percentage. For the calculation of the IRR the following equations were used:

\[ \sum_{i=0}^{n} C_F \cdot D_i = 0 \]  

where  
\[ C_F = \text{cash flow} \]  
\[ D_i = \text{discount factor in year i} \]  
\[ n = \text{plant life} \]  
\[ [\text{S/year}] \]

The cash flow equals:

\[ C_F = W + A \]  

where  
\[ A = \text{depreciation} \]  
\[ [\text{S/year}] \]
The discount factor is given by:
\[ D_i = (1 + \frac{IRR}{100\%})^{-i} \]

where \( IRR \) = internal rate of return

The depreciation equals: \( A = 1/10 \times I_f = 3.6 \) M$/year

where \( I_f = 0.8 \times I_T = 36.24 \) M$

The cash flow then becomes 8.42 M$/year

The residual value after depreciation is: \( s = 0.1 \times I_T = 4.53 \) M$

With the in/out ratio of the net cash flow (NCF) and of the 40% discount cash flow (DCF) the IRR was obtained from Figure V-7, Montfort (1991). With this value the in/out ratio should equal 1. The calculations are shown in Table H.5. This resulted in an internal rate of return of:

\[ IRR = 13\% \]

<table>
<thead>
<tr>
<th>Year</th>
<th>N.C.F [M$]</th>
<th>D.C.F. - 40% [M$]</th>
<th>IRR - 13% [M$]</th>
<th>( D_i ) 40%</th>
<th>( D_i ) 13%</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>45.30</td>
<td>45.30</td>
<td>45.30</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>1</td>
<td>8.42</td>
<td>6.02</td>
<td>7.45</td>
<td>0.71</td>
<td>0.88</td>
</tr>
<tr>
<td>2</td>
<td>8.42</td>
<td>4.30</td>
<td>6.60</td>
<td>0.51</td>
<td>0.78</td>
</tr>
<tr>
<td>3</td>
<td>8.42</td>
<td>3.07</td>
<td>5.84</td>
<td>0.36</td>
<td>0.69</td>
</tr>
<tr>
<td>4</td>
<td>8.42</td>
<td>2.19</td>
<td>5.17</td>
<td>0.26</td>
<td>0.61</td>
</tr>
<tr>
<td>5</td>
<td>8.42</td>
<td>1.57</td>
<td>4.57</td>
<td>0.19</td>
<td>0.54</td>
</tr>
<tr>
<td>6</td>
<td>8.42</td>
<td>1.12</td>
<td>4.05</td>
<td>0.13</td>
<td>0.48</td>
</tr>
<tr>
<td>7</td>
<td>8.42</td>
<td>0.80</td>
<td>3.58</td>
<td>0.10</td>
<td>0.43</td>
</tr>
<tr>
<td>8</td>
<td>8.42</td>
<td>0.57</td>
<td>3.17</td>
<td>0.07</td>
<td>0.38</td>
</tr>
<tr>
<td>9</td>
<td>8.42</td>
<td>0.41</td>
<td>2.80</td>
<td>0.05</td>
<td>0.33</td>
</tr>
<tr>
<td>10</td>
<td>12.9</td>
<td>0.29</td>
<td>2.48</td>
<td>0.02</td>
<td>0.19</td>
</tr>
<tr>
<td></td>
<td>5</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>In/out ratio</td>
<td>1.96</td>
<td>0.45</td>
<td>1.01</td>
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<td></td>
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</table>
## Appendix K

### Specification forms

<table>
<thead>
<tr>
<th>Component</th>
<th>Page</th>
</tr>
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<tbody>
<tr>
<td>Reactor R23</td>
<td>K-1</td>
</tr>
<tr>
<td>Distillation column T1</td>
<td>K-2</td>
</tr>
<tr>
<td>Distillation column T7</td>
<td>K-3</td>
</tr>
<tr>
<td>Distillation column T16</td>
<td>K-4</td>
</tr>
<tr>
<td>Aircoolers H2, H9 and H17</td>
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</tr>
<tr>
<td>Heat exchanger H3</td>
<td>K-6</td>
</tr>
<tr>
<td>Heat exchanger H6</td>
<td>K-7</td>
</tr>
<tr>
<td>Heat exchanger H15</td>
<td>K-8</td>
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<tr>
<td>Heat exchanger H18</td>
<td>K-9</td>
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<tr>
<td>Heat exchanger H24</td>
<td>K-10</td>
</tr>
<tr>
<td>Heat exchanger H25</td>
<td>K-11</td>
</tr>
<tr>
<td>Heat exchanger H28</td>
<td>K-12</td>
</tr>
<tr>
<td>Fired heater F20</td>
<td>K-13</td>
</tr>
<tr>
<td>Vessels V4, V12, V21 and V29</td>
<td>K-14</td>
</tr>
<tr>
<td>Pumps and compressors P10, P11, C19, P26 and P27</td>
<td>K-15</td>
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## Specification form reactor R23

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow</td>
<td>[kg/h]</td>
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</tr>
<tr>
<td>LHSV</td>
<td>[h⁻¹]</td>
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</tr>
<tr>
<td>Reactor height</td>
<td>[mm]</td>
<td>6,000</td>
</tr>
<tr>
<td>Reactor diameter</td>
<td>[mm]</td>
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</tr>
<tr>
<td>Superficial velocity</td>
<td>[m/s]</td>
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</tr>
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<td>[°C]</td>
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<tr>
<td>Temperature out</td>
<td>[°C]</td>
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</tr>
<tr>
<td>Pressure in</td>
<td>[bar G]</td>
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</tr>
<tr>
<td>Pressure drop</td>
<td>[mbar]</td>
<td>490</td>
</tr>
<tr>
<td>Catalyst type</td>
<td></td>
<td>Leuna Kontakt 8835</td>
</tr>
<tr>
<td>Catalyst shape</td>
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<td>Spherical</td>
</tr>
<tr>
<td>Catalyst diameter</td>
<td>[mm]</td>
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</tr>
<tr>
<td>Porosity</td>
<td>[-]</td>
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</tr>
<tr>
<td>Mass catalyst</td>
<td>[kg]</td>
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### Specification form distillation column T1

<table>
<thead>
<tr>
<th>Design</th>
<th>HETP [m]</th>
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<tr>
<td>Type of column</td>
<td>Packed</td>
<td>Column diameter [mm]</td>
</tr>
<tr>
<td>Number of theoretical stages [-]</td>
<td>73</td>
<td>Column height [mm]</td>
</tr>
<tr>
<td>Feedstage</td>
<td>6</td>
<td>Volume packing [m³]</td>
</tr>
<tr>
<td>Number of redistributors [-]</td>
<td>5</td>
<td>Height packing [mm]</td>
</tr>
<tr>
<td>Type of packing</td>
<td>Sulzer Mellapak 250X</td>
<td>Pressure drop [mbar]</td>
</tr>
<tr>
<td>Packing material</td>
<td>Carbon steel</td>
<td>Reflux ratio [-]</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operating conditions</th>
<th>Feed</th>
<th>Distillate</th>
<th>Bottom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature [°C]</td>
<td>142</td>
<td>139</td>
<td>152</td>
</tr>
<tr>
<td>Pressure [bar G]</td>
<td>0.1</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
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<td>757.3</td>
<td>760.4</td>
</tr>
<tr>
<td>Mass flow [kg/h]</td>
<td>60,112</td>
<td>55,792</td>
<td>4,319</td>
</tr>
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</table>

<table>
<thead>
<tr>
<th>Composition [wt%]</th>
<th>Feed</th>
<th>Distillate</th>
<th>Bottom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Methane</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Propane</td>
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<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Benzene</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Toluene</td>
<td>0.3</td>
<td>0.3</td>
<td>0.0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>6.6</td>
<td>7.1</td>
<td>0.0</td>
</tr>
<tr>
<td>para-Xylene</td>
<td>22.5</td>
<td>24.2</td>
<td>0.1</td>
</tr>
<tr>
<td>meta-Xylene</td>
<td>51.0</td>
<td>54.9</td>
<td>0.7</td>
</tr>
<tr>
<td>ortho-Xylene</td>
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<td>0.0</td>
<td>1.8</td>
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<td>1,2,4-Trimethylbenzene</td>
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<td>0.0</td>
<td>1.9</td>
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<tr>
<td>para-Diethylbenzene</td>
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<td>0.0</td>
<td>1.8</td>
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### Specification form distillation column T7

<table>
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</thead>
<tbody>
<tr>
<td>Type of column</td>
<td>Packed</td>
</tr>
<tr>
<td>Number of theoretical stages</td>
<td>[-]</td>
</tr>
<tr>
<td>Number of redistributors</td>
<td>[-]</td>
</tr>
<tr>
<td>Feedstage</td>
<td>31</td>
</tr>
<tr>
<td>Pressure drop [mbar]</td>
<td>107</td>
</tr>
<tr>
<td>Reflux ratio [-]</td>
<td>6.65</td>
</tr>
<tr>
<td>Column diameter [mm]</td>
<td>1,340</td>
</tr>
<tr>
<td>Retification [mm]</td>
<td>1,960</td>
</tr>
<tr>
<td>Stripping [mm]</td>
<td></td>
</tr>
<tr>
<td>Column height [mm]</td>
<td>37,000</td>
</tr>
<tr>
<td>Volume packing [m³]</td>
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</tr>
<tr>
<td>Height packing [mm]</td>
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<tr>
<td>Rectification [mm]</td>
<td></td>
</tr>
<tr>
<td>Stripping [mm]</td>
<td>10,000</td>
</tr>
<tr>
<td>Type of packing</td>
<td>Sulzer Mellapak 250X</td>
</tr>
<tr>
<td>Packing material</td>
<td>Carbon steel</td>
</tr>
<tr>
<td>Heating</td>
<td>Thermosyphon reboiler</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operating conditions</th>
<th>Feed</th>
<th>Distillate</th>
<th>Bottom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature [°C]</td>
<td>48</td>
<td>71</td>
<td>144</td>
</tr>
<tr>
<td>Pressure [bar G]</td>
<td>0.1</td>
<td>0.0</td>
<td>0.1</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>150.2</td>
<td>2.1</td>
<td>753.7</td>
</tr>
<tr>
<td>Mass flow [kg/h]</td>
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<td>2,978</td>
<td>43,862</td>
</tr>
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<td>Composition [wt%]</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td>0.0</td>
<td>0.1</td>
<td>0.0</td>
</tr>
<tr>
<td>Methane</td>
<td>0.0</td>
<td>0.4</td>
<td>0.0</td>
</tr>
<tr>
<td>Ethane</td>
<td>0.7</td>
<td>12.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Propane</td>
<td>0.7</td>
<td>10.6</td>
<td>0.0</td>
</tr>
<tr>
<td>Benzene</td>
<td>4.1</td>
<td>63.9</td>
<td>0.0</td>
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<tr>
<td>Toluene</td>
<td>0.8</td>
<td>11.4</td>
<td>0.0</td>
</tr>
<tr>
<td>Ethylbenzene</td>
<td>2.9</td>
<td>0.5</td>
<td>3.1</td>
</tr>
<tr>
<td>para-Xylene</td>
<td>21.6</td>
<td>0.5</td>
<td>23.0</td>
</tr>
<tr>
<td>meta-Xylene</td>
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<td>50.6</td>
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<td>21.2</td>
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<td>22.7</td>
</tr>
<tr>
<td>Cumene</td>
<td>0.2</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>1,2,4-Trimethylbenzene</td>
<td>0.2</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>para-Diethylbenzene</td>
<td>0.2</td>
<td>0.0</td>
<td>0.2</td>
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</table>
## Specification form distillation column T16

### Design

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<th>Type of column</th>
<th>Packed</th>
<th>HETP</th>
<th>Column diameter</th>
<th>Column height</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of theoretical</td>
<td></td>
<td>[m]</td>
<td>[mm]</td>
<td>[mm]</td>
</tr>
<tr>
<td>stages</td>
<td>HETP</td>
<td>0.5</td>
<td>1,290</td>
<td>54,500</td>
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<tr>
<td>Feedstage</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Number of</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>redistributors</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Type of packing</td>
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<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>250X Reboiler</td>
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<td></td>
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</tr>
<tr>
<td>Packing material</td>
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<td></td>
<td></td>
<td></td>
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### Operating conditions

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<tr>
<th>Condition</th>
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<th>Bottom</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature [°C]</td>
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<td>144</td>
<td>169</td>
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<tr>
<td>Pressure [bar G]</td>
<td>0.2</td>
<td>0.0</td>
<td>0.2</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>760.4</td>
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<td>736.4</td>
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<td>Mass flow [kg/h]</td>
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<td>4,044</td>
<td>275</td>
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</table>

| Composition [wt%]       |      |            |        |
| Hydrogen                | 0.0  | 0.0        | 0.0    |
| Methane                 | 0.0  | 0.0        | 0.0    |
| Ethane                  | 0.0  | 0.0        | 0.0    |
| Propane                 | 0.0  | 0.0        | 0.0    |
| Benzene                 | 0.0  | 0.0        | 0.0    |
| Toluene                 | 0.0  | 0.0        | 0.0    |
| Ethylbenzene            | 0.0  | 0.0        | 0.0    |
| para-Xylene             | 0.1  | 0.1        | 0.0    |
| meta-Xylene             | 0.7  | 0.8        | 0.0    |
| ortho-Xylene            | 93.7 | 99.1       | 14.7   |
| Cumene                  | 1.8  | 0.0        | 28.8   |
| 1,2,4-Trimethylbenzene  | 1.9  | 0.0        | 27.7   |
| para-Diethylbenzene     | 1.8  | 0.0        | 28.8   |
### Specification form aircoolers

<table>
<thead>
<tr>
<th>Unit number</th>
<th>H2</th>
<th>H9</th>
<th>H17</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat duty</td>
<td>14.68</td>
<td>2.06</td>
<td>2.10</td>
</tr>
<tr>
<td>Fluid temp</td>
<td>139.1</td>
<td>70.9</td>
<td>144.2</td>
</tr>
<tr>
<td>Air temp out</td>
<td>62.5</td>
<td>45.5</td>
<td>63.8</td>
</tr>
<tr>
<td>ΔT&lt;sub&gt;in&lt;/sub&gt;</td>
<td>88.7</td>
<td>29.4</td>
<td>93.1</td>
</tr>
<tr>
<td>Heat transfer area</td>
<td>718.5</td>
<td>318.3</td>
<td>104.0</td>
</tr>
<tr>
<td>Tube length</td>
<td>9,150</td>
<td>12,200</td>
<td>7,320</td>
</tr>
<tr>
<td>Tube diameter</td>
<td>25.4</td>
<td>25.4</td>
<td>25.4</td>
</tr>
<tr>
<td>Mass flow</td>
<td>175,257</td>
<td>22,908</td>
<td>24,925</td>
</tr>
<tr>
<td>Pressure drop fluid</td>
<td>47</td>
<td>18</td>
<td>25</td>
</tr>
<tr>
<td>Fan power</td>
<td>88.24</td>
<td>39.09</td>
<td>12.77</td>
</tr>
</tbody>
</table>
**Specification form heat exchanger H3**

### General characteristics

<table>
<thead>
<tr>
<th>Type</th>
<th>Reboiler</th>
</tr>
</thead>
<tbody>
<tr>
<td>Configuration</td>
<td>Thermosyphon</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Heat duty [Gcal/h]</td>
<td>14.62</td>
</tr>
<tr>
<td>Heat transfer area [m²]</td>
<td>404.8</td>
</tr>
<tr>
<td>Design heat flux [kcal/h/m²]</td>
<td>36,113</td>
</tr>
<tr>
<td>$\Delta T_{in}$ [°C]</td>
<td>39.95</td>
</tr>
<tr>
<td>Correction factor $\Delta T_{in}$ [-]</td>
<td>1.0</td>
</tr>
<tr>
<td>Corrected $\Delta T_{in}$ [°C]</td>
<td>39.95</td>
</tr>
<tr>
<td>Number of passes tube-side [-]</td>
<td>1</td>
</tr>
<tr>
<td>Number of passes shell-side [-]</td>
<td>1</td>
</tr>
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</table>

### Operating conditions

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Shell-side</th>
<th>Tube-side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow [kg/h]</td>
<td>175,716</td>
<td>47,772</td>
</tr>
<tr>
<td>Specific heat in [kcal/kg/°C]</td>
<td>0.53</td>
<td>0.66</td>
</tr>
<tr>
<td>Temperature in [°C]</td>
<td>151.8</td>
<td>191.7</td>
</tr>
<tr>
<td>Temperature out [°C]</td>
<td>151.8</td>
<td>191.7</td>
</tr>
<tr>
<td>Pressure in [bar G]</td>
<td>0.2</td>
<td>12.0</td>
</tr>
<tr>
<td>Pressure drop [mbar]</td>
<td>50</td>
<td>0.0</td>
</tr>
<tr>
<td>Construction material</td>
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<td>Carbon steel</td>
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## Specification form heat exchanger H6

### General characteristics

<table>
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<th>Type</th>
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<tbody>
<tr>
<td>Configuration</td>
<td>Thermosyphon</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Heat duty</td>
<td>[Gcal/h] 4.25</td>
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<tr>
<td>Heat transfer area</td>
<td>[m²] 95.09</td>
</tr>
<tr>
<td>Design heat flux</td>
<td>[kcal/h/m²] 44,712</td>
</tr>
<tr>
<td>ΔT_in</td>
<td>[°C] 49.93</td>
</tr>
<tr>
<td>Correction factor ΔT_in</td>
<td>[-] 1.0</td>
</tr>
<tr>
<td>Corrected ΔT_in</td>
<td>[°C] 49.93</td>
</tr>
<tr>
<td>Number of passes tube-side</td>
<td>[-] 1</td>
</tr>
<tr>
<td>Number of passes shell-side</td>
<td>[-] 1</td>
</tr>
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### Operating conditions

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Shell-side</th>
<th>Tube-side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid</td>
<td>Bottom T7</td>
<td>Steam</td>
</tr>
<tr>
<td>Mass flow</td>
<td>[kg/h] 51,264</td>
<td>13,896</td>
</tr>
<tr>
<td>Specific heat in</td>
<td>[kcal/kg/°C] 0.52</td>
<td>0.66</td>
</tr>
<tr>
<td>Temperature in</td>
<td>[°C] 141.8</td>
<td>191.7</td>
</tr>
<tr>
<td>Temperature out</td>
<td>[°C] 141.8</td>
<td>191.7</td>
</tr>
<tr>
<td>Pressure in</td>
<td>[bar G] 0.0</td>
<td>12.0</td>
</tr>
<tr>
<td>Pressure drop</td>
<td>[mbar] 70</td>
<td>0.0</td>
</tr>
<tr>
<td>Construction material</td>
<td>Carbon steel</td>
<td>Carbon steel</td>
</tr>
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</table>
# Specification form heat exchanger H15

## General characteristics

<table>
<thead>
<tr>
<th>Type</th>
<th>Integrated heat exchanger</th>
</tr>
</thead>
<tbody>
<tr>
<td>Configuration</td>
<td>Floating head</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Heat duty [Gcal/h]</td>
<td>9.08</td>
</tr>
<tr>
<td>Heat transfer area [m²]</td>
<td>120.3</td>
</tr>
<tr>
<td>Overall heat transfer coeff. [kcal/h/m²°C]</td>
<td>427</td>
</tr>
<tr>
<td>ΔT₁m [°C]</td>
<td>177.1</td>
</tr>
<tr>
<td>Correction factor ΔT₁m [-]</td>
<td>1.0</td>
</tr>
<tr>
<td>Corrected ΔT₁m [°C]</td>
<td>177.1</td>
</tr>
<tr>
<td>Number of passes tube-side [-]</td>
<td>1</td>
</tr>
<tr>
<td>Number of passes shell-side [-]</td>
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## Operating conditions

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Shell-side</th>
<th>Tube-side</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Reactor feed</td>
<td>Reactor effluent</td>
</tr>
<tr>
<td>Mass flow [kg/h]</td>
<td>66,204</td>
<td>66,204</td>
</tr>
<tr>
<td>Mass flow to be evaporated [kg/h]</td>
<td>48,060</td>
<td>-</td>
</tr>
<tr>
<td>Specific heat in [kcal/kg/°C]</td>
<td>0.69</td>
<td>0.66</td>
</tr>
<tr>
<td>Temperature in [°C]</td>
<td>48.9</td>
<td>398.9</td>
</tr>
<tr>
<td>Temperature out [°C]</td>
<td>182.9</td>
<td>192.9</td>
</tr>
<tr>
<td>Pressure in [bar G]</td>
<td>8.59</td>
<td>7.0</td>
</tr>
<tr>
<td>Pressure drop [mbar]</td>
<td>600</td>
<td>20</td>
</tr>
<tr>
<td>Construction material</td>
<td>Carbon steel</td>
<td>Carbon steel</td>
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### General characteristics

<table>
<thead>
<tr>
<th>Type</th>
<th>Reboiler</th>
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<tbody>
<tr>
<td>Configuration</td>
<td>Thermosyphon</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Heat duty</td>
<td>[Gcal/h] 8.75</td>
</tr>
<tr>
<td>Heat transfer area</td>
<td>[m²] 115.8</td>
</tr>
<tr>
<td>Design heat flux</td>
<td>[kcal/h/m²] 18,057</td>
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<tr>
<td>$\Delta T_{\text{min}}$</td>
<td>[$^\circ\text{C}$] 23.28</td>
</tr>
<tr>
<td>Correction factor $\Delta T_{\text{min}}$</td>
<td>[-] 1.0</td>
</tr>
<tr>
<td>Corrected $\Delta T_{\text{min}}$</td>
<td>[$^\circ\text{C}$] 23.28</td>
</tr>
<tr>
<td>Number of passes tube-side</td>
<td>[-] 1</td>
</tr>
<tr>
<td>Number of passes shell-side</td>
<td>[-] 1</td>
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### Operating conditions

<table>
<thead>
<tr>
<th>Fluid</th>
<th>Shell-side</th>
<th>Tube-side</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Bottom T16</td>
<td>Steam</td>
</tr>
<tr>
<td>Mass flow</td>
<td>[kg/h] 26,280</td>
<td>6,840</td>
</tr>
<tr>
<td>Specific heat in</td>
<td>[kcal/kg/$^\circ\text{C}$] 0.55</td>
<td>0.66</td>
</tr>
<tr>
<td>Temperature in</td>
<td>[$^\circ\text{C}$] 168.5</td>
<td>191.7</td>
</tr>
<tr>
<td>Temperature out</td>
<td>[$^\circ\text{C}$] 168.5</td>
<td>191.7</td>
</tr>
<tr>
<td>Pressure in</td>
<td>[bar G] 0.2</td>
<td>12.0</td>
</tr>
<tr>
<td>Pressure drop</td>
<td>[mbar] 10</td>
<td>0.0</td>
</tr>
<tr>
<td>Construction material</td>
<td>Carbon steel</td>
<td>Carbon steel</td>
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## Specification form heat exchanger H24

### General characteristics

<table>
<thead>
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<th>Heat exchanger</th>
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<tbody>
<tr>
<td>Type</td>
<td>Heat exchanger</td>
</tr>
<tr>
<td>Configuration</td>
<td>Floating head</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Heat duty [Gcal/h]</td>
<td>0.22</td>
</tr>
<tr>
<td>Heat transfer area [m²]</td>
<td>24.94</td>
</tr>
<tr>
<td>Overall heat transfer coeff. [kcal/h/m²/°C]</td>
<td>298</td>
</tr>
<tr>
<td>ΔT_in [°C]</td>
<td>29.75</td>
</tr>
<tr>
<td>Correction factor ΔT_in [-]</td>
<td>0.98</td>
</tr>
<tr>
<td>Corrected ΔT_in [°C]</td>
<td>29.15</td>
</tr>
<tr>
<td>Number of passes tube-side [-]</td>
<td>4</td>
</tr>
<tr>
<td>Number of passes shell-side [-]</td>
<td>1</td>
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</table>

### Operating conditions

<table>
<thead>
<tr>
<th></th>
<th>Shell-side</th>
<th>Tube-side</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fluid</td>
<td>ortho-Xylene product</td>
<td>Water</td>
</tr>
<tr>
<td>Mass flow [kg/h]</td>
<td>4,032</td>
<td>30,960</td>
</tr>
<tr>
<td>Specific heat in [kcal/kg/°C]</td>
<td>0.47</td>
<td>1.00</td>
</tr>
<tr>
<td>Temperature in [°C]</td>
<td>144.2</td>
<td>27.0</td>
</tr>
<tr>
<td>Temperature out [°C]</td>
<td>30.0</td>
<td>34.0</td>
</tr>
<tr>
<td>Pressure in [bar G]</td>
<td>-0.1</td>
<td>3.5</td>
</tr>
<tr>
<td>Pressure drop [mbar]</td>
<td>110</td>
<td>880</td>
</tr>
<tr>
<td>Construction material</td>
<td>Carbon steel</td>
<td>Carbon steel</td>
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## Specification form heat exchanger H25

### General characteristics

<table>
<thead>
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<th>Type</th>
<th>Heat exchanger</th>
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<tbody>
<tr>
<td>Configuration</td>
<td>Floating head</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
</tr>
<tr>
<td>Heat duty $[\text{Gcal/h}]$</td>
<td>0.02</td>
</tr>
<tr>
<td>Heat transfer area $[\text{m}^2]$</td>
<td>1.58</td>
</tr>
<tr>
<td>Overall heat transfer coeff. $[\text{kcal/h/m}^2/\text{oC}]$</td>
<td>217</td>
</tr>
<tr>
<td>$\Delta T_{\text{in}}$ $[^\circ \text{C}]$</td>
<td>51.96</td>
</tr>
<tr>
<td>Correction factor $\Delta T_{\text{in}}$ [-]</td>
<td>0.98</td>
</tr>
<tr>
<td>Corrected $\Delta T_{\text{in}}$ $[^\circ \text{C}]$</td>
<td>50.92</td>
</tr>
<tr>
<td>Number of passes tube-side [-]</td>
<td>6</td>
</tr>
<tr>
<td>Number of passes shell-side [-]</td>
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</tbody>
</table>

### Operating conditions

<table>
<thead>
<tr>
<th>Fluid</th>
<th>C$_9$ stream</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow $[\text{kg/h}]$</td>
<td>252</td>
<td>2,484</td>
</tr>
<tr>
<td>Specific heat in $[\text{kcal/kg/}^\circ \text{C}]$</td>
<td>0.49</td>
<td>1.00</td>
</tr>
<tr>
<td>Temperature in $[^\circ \text{C}]$</td>
<td>168.5</td>
<td>27.0</td>
</tr>
<tr>
<td>Temperature out $[^\circ \text{C}]$</td>
<td>40.0</td>
<td>34.0</td>
</tr>
<tr>
<td>Pressure in $[\text{bar G}]$</td>
<td>0.2</td>
<td>3.5</td>
</tr>
<tr>
<td>Pressure drop $[\text{mbar}]$</td>
<td>10</td>
<td>650</td>
</tr>
<tr>
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<td>Carbon steel</td>
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### General characteristics

<table>
<thead>
<tr>
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<th>Condenser</th>
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<tbody>
<tr>
<td><strong>Type</strong></td>
<td>Condenser</td>
</tr>
<tr>
<td><strong>Configuration</strong></td>
<td>Floating head</td>
</tr>
<tr>
<td><strong>Position</strong></td>
<td>Horizontal</td>
</tr>
<tr>
<td><strong>Heat duty</strong> [Gcal/h]</td>
<td>9.40</td>
</tr>
<tr>
<td><strong>Heat transfer area</strong> [m²]</td>
<td>386.5</td>
</tr>
<tr>
<td><strong>Overall heat transfer coeff.</strong> [kcal/h/m²/°C]</td>
<td>354.5</td>
</tr>
<tr>
<td>∆Tₗₘ [°C]</td>
<td>69.3</td>
</tr>
<tr>
<td>Correction factor ∆Tₗₘ [-]</td>
<td>0.99</td>
</tr>
<tr>
<td>Corrected ∆Tₗₘ [°C]</td>
<td>68.6</td>
</tr>
<tr>
<td><strong>Number of passes tube-side</strong> [-]</td>
<td>2</td>
</tr>
<tr>
<td><strong>Number of passes shell-side</strong> [-]</td>
<td>1</td>
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### Operating conditions

<table>
<thead>
<tr>
<th></th>
<th>Shell-side</th>
<th>Tube-side</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Fluid</strong></td>
<td>Reactor effluent</td>
<td>Water</td>
</tr>
<tr>
<td><strong>Mass flow</strong> [kg/h]</td>
<td>66,204</td>
<td>1,345,356</td>
</tr>
<tr>
<td><strong>Mass flow to be condensed</strong> [kg/h]</td>
<td>46,836</td>
<td>-</td>
</tr>
<tr>
<td><strong>Specific heat in</strong> [kcal/kg/°C]</td>
<td>0.67</td>
<td>1.00</td>
</tr>
<tr>
<td><strong>Temperature in</strong> [°C]</td>
<td>193.1</td>
<td>27.0</td>
</tr>
<tr>
<td><strong>Temperature out</strong> [°C]</td>
<td>48.9</td>
<td>34.0</td>
</tr>
<tr>
<td><strong>Pressure in</strong> [bar G]</td>
<td>7.0</td>
<td>3.5</td>
</tr>
<tr>
<td><strong>Pressure drop</strong> [mbar]</td>
<td>97</td>
<td>360</td>
</tr>
<tr>
<td><strong>Construction material</strong></td>
<td>Carbon steel</td>
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</tr>
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</table>
### Specification form fired heater F20

<table>
<thead>
<tr>
<th>Type of fired heater</th>
<th>Vertical cylindrical fired heater</th>
</tr>
</thead>
<tbody>
<tr>
<td>LHV fuel gas ([\text{kcal/Nm}^3])</td>
<td>8,870</td>
</tr>
<tr>
<td>Fuel consumed ([\text{kg/h}])</td>
<td>772</td>
</tr>
<tr>
<td>Excess air ([%])</td>
<td>20</td>
</tr>
<tr>
<td>Pressure drop ([\text{mbar}])</td>
<td>500</td>
</tr>
<tr>
<td>Mass flow ([\text{kg/h}])</td>
<td>66,198</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Section</th>
<th>Radiant section</th>
<th>Convection section</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Shield bank</td>
<td>Fin bank</td>
</tr>
<tr>
<td>Temperature in ([\text{°C}])</td>
<td>260</td>
<td>254</td>
</tr>
<tr>
<td>Temperature out ([\text{°C}])</td>
<td>395</td>
<td>260</td>
</tr>
<tr>
<td>Heat absorbed ([\text{Gcal/h}])</td>
<td>6.7</td>
<td>1.0</td>
</tr>
<tr>
<td>Number of tubes ([-])</td>
<td>60</td>
<td>60</td>
</tr>
<tr>
<td>Number of passes ([-])</td>
<td>20</td>
<td>20</td>
</tr>
<tr>
<td>Tube length ([\text{mm}])</td>
<td>10,360</td>
<td>3,350</td>
</tr>
<tr>
<td>Tube diameter ([\text{mm}])</td>
<td>102</td>
<td>102</td>
</tr>
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## Specification form vessels

<table>
<thead>
<tr>
<th>Unit number</th>
<th>V4</th>
<th>V12</th>
<th>V21</th>
<th>V29</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unit type</td>
<td>Reflux drum</td>
<td>Gas/liquid separator</td>
<td>Reflux drum</td>
<td>Gas/liquid separator</td>
</tr>
<tr>
<td>Position</td>
<td>Horizontal</td>
<td>Horizontal</td>
<td>Horizontal</td>
<td>Vertical</td>
</tr>
<tr>
<td>Process fluid</td>
<td>Top T1</td>
<td>Top T7</td>
<td>Top T16</td>
<td>Cooled reactor effluent</td>
</tr>
<tr>
<td>Pressure [bar G]</td>
<td>0.0</td>
<td>0.0</td>
<td>0.0</td>
<td>6.9</td>
</tr>
<tr>
<td>Temperature [°C]</td>
<td>141</td>
<td>96</td>
<td>145</td>
<td>49</td>
</tr>
<tr>
<td>Volume [m³]</td>
<td>42.8</td>
<td>5.1</td>
<td>6.3</td>
<td>13.1</td>
</tr>
<tr>
<td>Diameter [mm]</td>
<td>2,390</td>
<td>1,000</td>
<td>1,260</td>
<td>1,730</td>
</tr>
<tr>
<td>Height [mm]</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>5,590</td>
</tr>
<tr>
<td>Length [mm]</td>
<td>9,540</td>
<td>6,430</td>
<td>5,020</td>
<td>-</td>
</tr>
<tr>
<td>Liquid height [mm]</td>
<td>1,200</td>
<td>750</td>
<td>630</td>
<td>3,350</td>
</tr>
<tr>
<td>Construction material</td>
<td>carbon steel</td>
<td>carbon steel</td>
<td>carbon steel</td>
<td>carbon steel</td>
</tr>
<tr>
<td>Special features</td>
<td></td>
<td></td>
<td></td>
<td>demister installed</td>
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# Specification form pumps and compressors

<table>
<thead>
<tr>
<th>Unit number</th>
<th>P10</th>
<th>P11</th>
<th>C19</th>
<th>P26</th>
<th>P27</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unit type</td>
<td>Pump</td>
<td>Pump</td>
<td>Compressor</td>
<td>Pump</td>
<td>Pump</td>
</tr>
<tr>
<td>Process fluid</td>
<td>Bottom T3</td>
<td>Crystallization filtrate</td>
<td>Gas recycle</td>
<td>Top T16</td>
<td>Bottom T16</td>
</tr>
<tr>
<td>Mass flow [kg/h]</td>
<td>43,862</td>
<td>46,899</td>
<td>18,393</td>
<td>4,044</td>
<td>275.0</td>
</tr>
<tr>
<td>Density [kg/m³]</td>
<td>753.7</td>
<td>857.8</td>
<td>3.09</td>
<td>870.7</td>
<td>851.7</td>
</tr>
<tr>
<td>Pressure in [bar G]</td>
<td>0.1</td>
<td>4.0</td>
<td>6.9</td>
<td>-0.2</td>
<td>0.2</td>
</tr>
<tr>
<td>Pressure out [bar G]</td>
<td>0.6</td>
<td>8.6</td>
<td>8.6</td>
<td>4.0</td>
<td>4.0</td>
</tr>
<tr>
<td>Efficiency [-]</td>
<td>0.75</td>
<td>0.75</td>
<td>0.75</td>
<td>0.50</td>
<td>0.50</td>
</tr>
<tr>
<td>Power [kW]</td>
<td>1.1</td>
<td>9.3</td>
<td>347.1</td>
<td>1.1</td>
<td>0.1</td>
</tr>
<tr>
<td>T_{in} [°C]</td>
<td>144</td>
<td>30</td>
<td>49</td>
<td>30</td>
<td>40</td>
</tr>
<tr>
<td>T_{out} [°C]</td>
<td>144</td>
<td>30</td>
<td>68</td>
<td>30</td>
<td>40</td>
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</tbody>
</table>

The reflux pumps P5, P13 and P22 were not designed.
Appendix L

Effects of an additional adsorption unit
Effects of an additional adsorption unit

### Table L.1  Heat duties and pump and compressor powers of situation 1 and situation 2

<table>
<thead>
<tr>
<th>Unit</th>
<th></th>
<th>situation 1</th>
<th>situation 2</th>
<th>relative decrease %</th>
</tr>
</thead>
<tbody>
<tr>
<td>H2</td>
<td>heat duty [Gcal/h]</td>
<td>14.67</td>
<td>14.57</td>
<td>0.7</td>
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<tr>
<td>H3</td>
<td>heat duty [Gcal/h]</td>
<td>14.62</td>
<td>14.53</td>
<td>0.6</td>
</tr>
<tr>
<td>H6</td>
<td>heat duty [Gcal/h]</td>
<td>4.32</td>
<td>3.98</td>
<td>7.8</td>
</tr>
<tr>
<td>H9</td>
<td>heat duty [Gcal/h]</td>
<td>2.06</td>
<td>1.84</td>
<td>10.5</td>
</tr>
<tr>
<td>H15</td>
<td>heat duty [Gcal/h]</td>
<td>9.09</td>
<td>8.91</td>
<td>2.0</td>
</tr>
<tr>
<td>H17</td>
<td>heat duty [Gcal/h]</td>
<td>2.10</td>
<td>1.94</td>
<td>7.7</td>
</tr>
<tr>
<td>H18</td>
<td>heat duty [Gcal/h]</td>
<td>2.09</td>
<td>1.93</td>
<td>7.8</td>
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<tr>
<td>H24</td>
<td>heat duty [Gcal/h]</td>
<td>0.22</td>
<td>0.21</td>
<td>4.9</td>
</tr>
<tr>
<td>H25</td>
<td>heat duty [Gcal/h]</td>
<td>0.02</td>
<td>0.02</td>
<td>8.3</td>
</tr>
<tr>
<td>H28</td>
<td>heat duty [Gcal/h]</td>
<td>9.39</td>
<td>9.21</td>
<td>1.8</td>
</tr>
<tr>
<td>F20</td>
<td>heat absorbed [Gcal/h]</td>
<td>9.32</td>
<td>9.08</td>
<td>2.5</td>
</tr>
<tr>
<td>C20</td>
<td>power [kW]</td>
<td>347.10</td>
<td>349.36</td>
<td>-0.7</td>
</tr>
<tr>
<td>P10</td>
<td>power [kW]</td>
<td>1.08</td>
<td>0.98</td>
<td>9.1</td>
</tr>
<tr>
<td>P11</td>
<td>power [kW]</td>
<td>9.30</td>
<td>8.63</td>
<td>7.1</td>
</tr>
<tr>
<td>P26</td>
<td>power [kW]</td>
<td>1.09</td>
<td>1.04</td>
<td>4.9</td>
</tr>
<tr>
<td>P27</td>
<td>power [kW]</td>
<td>0.069</td>
<td>0.063</td>
<td>8.4</td>
</tr>
</tbody>
</table>

### Table L.2  Column diameters of situation 1 and situation 2

<table>
<thead>
<tr>
<th>Unit</th>
<th></th>
<th>situation 1</th>
<th>situation 2</th>
<th>relative decrease %</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1</td>
<td>column diameter [mm]</td>
<td>3440</td>
<td>3240</td>
<td>5.8</td>
</tr>
<tr>
<td>T7</td>
<td>column diameter top [mm]</td>
<td>1340</td>
<td>1280</td>
<td>4.5</td>
</tr>
<tr>
<td></td>
<td>column diameter bottom [mm]</td>
<td>1960</td>
<td>1880</td>
<td>4.1</td>
</tr>
<tr>
<td>T16</td>
<td>column diameter [mm]</td>
<td>1290</td>
<td>1250</td>
<td>3.1</td>
</tr>
</tbody>
</table>