FVO Nr. 3153

Preliminary Design Assignment
Department of Chemical Technology

Subject
Removal of SO₂ and NOₓ from flue gas using Interconnected Fluidized Beds and production of sulfur from the removed SO₂

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I.F.B., Superclaus, sulfur dioxide, nitrogen oxides, sulfur

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SUMMARY

The removal Unit of sulfur dioxide and nitrogen oxides consists of an IFB NOXSO Unit; The 'connect unit' consists of a reduction step of sulfur dioxide to hydrogen sulfide with hydrogen, a reduction step of carbon dioxide to methane with hydrogen and a tower section in which nearly all hydrogen sulfide and 52% of the carbon dioxide remaining in the process stream after the carbon dioxide reduction step are fed to the sulfur recovery unit. The sulfur recovery Unit consists of a superclaus plant.

The total sulfur production is 14589.2 tons a year or 39.97 tons a day. An ordinary sulfur plant is capable of producing 72 tons a day. Surely, the sulfur production capacity is large enough. The process however is not economically justified, because the Internal Rate of Return is -34.48% and the Return On Investment is -39.27%.

The goal to obtain a removal of 95% of the sulfur containing compounds is not accomplished. The total sulfur yield is 93.11%, this value is low compared to literature data, because chemical equilibria have been considered instead of selective catalytic reactions. This is done because the kinetics of the two catalytic claus reactors is unknown and because little is known about the kinetics of the superclaus unit.

The total yield of nitrogen oxides is 90% (as required in the assignment).

Comparing the emission standards for sulfur dioxide, carbon dioxide and nitrogen oxides with the actual stack massflows, it can be concluded that the emission standard of sulfur dioxide is exceeded. This is a result of the low sulfur recovery efficiency as mentioned above.
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This Preliminary Design Assignment (PDA) deals with a method to remove sulfur dioxide and nitrogen oxides from the flue gas of a 150 MWe power plant. This design is developed in cooperation with the American NOXSO corporation.

The process is based on a regenerative sorbent material that needs to be recirculated between the adsorber and the regenerator. For this purpose an Interconnected Fluidized Bed (IFB) reactor system is in development at the Delft University of Technology (DUT). In the IFB reactor system differential aeration is applied to obtain the driving force for solids circulation. The sorbent flows over a weir and through an orifice that connects the different compartments. The NOXSO corporation now is operating a plant which consists of fluidized beds connected by long pipes. In these pipes the loss of solid sorbent is significant. The IFB design offers an alternate route with less attrition. Transportation is achieved in a fluidized mode, thus reducing the loss of sorbent due to attrition.

This PDA consists of an IFB NOXSO Unit and a Sulfur Recovery Unit (SRU). The captured nitrogen oxides are recycled from the IFB NOXSO Unit to the 150 MWe power plant to reduce the amount of nitrogen oxides to be formed in the furnace of the power plant. In the SRU the captured sulfur dioxide is processed to a salable product. A superclaus installation is used because of the fact that it is well-known technology and the sulfur yield will be over 99% [3].

The designed plant should be able of removing at least 95% of the sulfur containing components and 90% of the nitrogen oxides. Furthermore the economics of the designed plant should make clear whether the plant is economically efficient. Also the total sulfur production of the designed plant should be compared with the sulfur production of ordinary superclaus plants (which is approximately 72 tons of sulfur per day). This way it will be known if it is reasonable to build a superclaus plant after the IFB NOXSO Unit.

The major reason for the efforts to build a plant that is capable of removing sulfur dioxides and nitrogen oxides from a gas stream is the environmental aspect. These substances are known sources of environmental pollution such as acid rain. The national and international standards for the emission of several chemical substances such as sulfur dioxide and nitrogen oxides will be more and more severe.

<table>
<thead>
<tr>
<th>Table 2.1. National emission standards in Holland</th>
</tr>
</thead>
<tbody>
<tr>
<td><img src="image" alt="Table" /></td>
</tr>
</tbody>
</table>

To meet these standards, it has been found by Cichanowicz [4] that the NOXSO process has the best starting-points in refer to the competitive processes such as flue gas desulfurization or selective catalytic reduction.
Process units:
1. regenerator
2. $\text{SO}_2$ reduction
3. Claus reactors
4. superclaus reactor
5. incinerator
6. furnace
7. Claus reactors
8. superclaus reactor
9. incinerator
10. $\text{CO}_2$ reduction
11. towers
12. Claus furnace
13. Claus reactors
14. superclaus reactor
15. incinerator

Figure 3.1 Process scheme of the different routes possible for the sulfur recovery
3. STARTING POINTS

3.1 CHOICE OF PROCESS ROUTE AND ROUGH DESCRIPTION OF CHOSEN ROUTE

The goal of this design is to develop a plant which can clean the flue gas originating from a 150 MWe power plant. The plant must be capable of reducing the amount sulfur containing substances and the nitrogen oxides in the stack with respectively 95% and 90%. The design has to be based on the NOXSO design and the NO\textsubscript{x} and SO\textsubscript{2} concentrations in the feed of the cleaning plant are listed in Table 3.1.

Table 3.1. Concentrations in flue gas entering the cleaning plant.

<table>
<thead>
<tr>
<th>Component</th>
<th>Volume</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[-]</td>
</tr>
<tr>
<td>NO\textsubscript{x}</td>
<td>500 [ppm]</td>
</tr>
<tr>
<td>SO\textsubscript{2}</td>
<td>2400 [Nm\textsuperscript{3}/s]</td>
</tr>
<tr>
<td>Total Flow</td>
<td>172.28</td>
</tr>
</tbody>
</table>

The part of the plant in which NO\textsubscript{x} and SO\textsubscript{2} are removed, cannot freely be chosen or designed in this preliminary design assignment. This part of the plant consists of an IFB Unit (IFB NOXSO Unit).

The IFB system can be splitted into four steps: the adsorber, the heater, the regenerator and the cooler. In the adsorber the NO\textsubscript{x} and the SO\textsubscript{2} are removed from the flue gas stream by adsorption on a solid sorbent. This sorbent consists of Na\textsubscript{2}O sites on a y-alumina carrier and the adsorption takes place as described by reactions (4.1), (4.2) and (4.3) in §4.3.1.1. The adsorption comes down to the forming of NO\textsubscript{x} ' and SO\textsubscript{2} on the sites of the sorbent.

In the heater the NO\textsubscript{x} is removed from the sorbent and sent back to the coal burner of the power station in order to suppress the formation of NO\textsubscript{x}.

The next step takes place in the regenerator. Here the sulfur containing compounds are removed from the sorbent. This process can be described by reactions (4.8), (4.9), (4.10) and (4.11) in §4.3.1.3. Here the SO\textsubscript{2} and SO\textsubscript{3} are removed from the sorbent sites by using natural gas. The products are SO\textsubscript{2} and H\textsubscript{2}S. Hydrogen could also be used however natural gas gives better results and is cheaper.

The final step in the IFB system is the cooler. The sorbent is cooled in the cooler and ready again for the adsorption step.
In the regenerator formed H$_2$S and SO$_2$ is fed to the Sulfur Recovery Unit. The main goal of the SRU is to obtain the highest possible conversion of sulfur dioxide to a salable product. In this preliminary design assignment it is chosen to produce sulfur (S$_3$-configuration) as a salable product. This restriction is made because of a shortage in time for a broader design. Another salable product could be sulphuric acid. The selection of the SRU configuration with the highest sulfur yield was done by comparing several different process routes with different units. Here, only different routes containing the superclaus steps will be examined. This will be done because superclaus processes are frequently used in the industrial processes in which sulfur is produced. So superclaus technology is well-known technology. Furthermore this is a process in which no water condensation (difficult, expensive) is needed and also no waste streams are produced.

The first step in the Sulfur Recovery Unit must be reduction of sulfur dioxide to hydrogen sulfide. The following process steps will depend on the degree of reduction of sulfur dioxide. For these following process steps two different process routes were examined (see Figure 3.1):

1) In case of reduction of sulfur dioxide to hydrogen sulfide, with a H$_2$S to SO$_2$ ratio of 2, it is possible according to Pearson [1] to lead the process stream directly into catalytic Claus reactors, with the accompanying condensors. Then the product stream enters a superclaus reactor.

2) In case of complete reduction of sulfurdioxide to hydrogen sulfide, a superclaus SRU consisting of a furnace and catalytic (super)Claus reactors will follow.

The main reactions which take place in the SRU are:

The reduction of sulfur dioxide is carried out with hydrogen; the main reactions are:

\[ 2 \text{SO}_2 + 4 \text{H}_2 \rightarrow 4 \text{H}_2\text{O} + \text{S}_2 \quad (3.1) \]

\[ 2 \text{H}_2 + \text{S}_2 \rightarrow 2 \text{H}_2\text{S} \quad (3.2) \]

These reactions are catalyzed by an activated bauxite catalyst.

The overall Claus reaction is:

\[ \text{H}_2\text{S} + \frac{1}{2} \text{O}_2 \rightarrow \frac{1}{2} \text{S}_8 + \text{H}_2\text{O} \quad (3.3) \]

This reaction is catalyzed by the Kaiser S-501 catalyst.

The overall reaction for the superclaus step is:

\[ \text{H}_2\text{S} + \frac{1}{2} \text{O}_2 \rightarrow \frac{1}{n} \text{S}_n + \text{H}_2\text{O} \quad (n=6-8) \quad (3.4) \]

This reaction is catalyzed by a sodium promoted 5 wt% iron oxide on silica catalyst and very selective.

3.2 OTHER SPECIFICATIONS AND SPECIALTIES OF THE PLANT

3.2.1 ADDITIVES FOR THE IFB UNIT

Additives used in this part of the plant are air, nitrogen, natural gas and steam. Air is obtained from the atmosphere, liquid nitrogen from storage tanks, liquid natural gas from storage tanks and steam from boiler feed water. The absorber material consists of Na$_2$O sites on a γ-alumina carrier.
3.2.2 ADDITIVES FOR SULFUR RECOVERY UNIT

Additives used here are hydrogen, steam and air. Again air and steam are obtained respectively from the atmosphere and from boiler feed water. Liquid hydrogen is obtained from storage tanks.

Catalysts used are activated bauxite catalyst (§4.2.2.1), nickel magnesium oxide on a γ-alumina support (§4.2.2.2), Kaiser S-501 (§4.2.3.4) and a sodium promoted 5 wt% iron oxide on a silica support (§4.2.3.5).

Furthermore stoneware raschig rings are used.

3.2.3 NON-PROCESSING ADDITIVES

Additives that are not part of the process stream but are used to cool or to heat the process stream are natural gas, steam (3 bar, 190 °C; 10 bar, 220 °C; 40 bar, 410 °C) and boiler feed water.

3.2.4 SPECIALTIES

The location of the plant cannot freely be chosen. The plant has to be built next to the electrical power plant its feed originates from.

3.3 PHYSICAL AND THERMODYNAMIC CONSTANTS

The physical constants used for the calculation of the heat capacities are given in table 3.3. To obtain the heat capacities formula (3.5) was used.

\[
C_p = a + b \cdot T + c \cdot T^2 + \frac{d}{T^2} \quad (3.5)
\]

Below a list of thermodynamic properties (table 3.2) of the process substances are presented as well.
Table 3.2. List of thermodynamic properties of the substances, present in the process

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2S$ (g)</td>
<td>34.1</td>
<td>-20.6</td>
<td>205.8</td>
<td>25.4</td>
<td>24.5</td>
<td>-4.0</td>
<td>1.70</td>
</tr>
<tr>
<td>$H_2$ (g)</td>
<td>2.0</td>
<td>0.0</td>
<td>130.7</td>
<td>31.4</td>
<td>-5.5</td>
<td>4.5</td>
<td>-1.1</td>
</tr>
<tr>
<td>$SO_2$ (g)</td>
<td>64.1</td>
<td>-296.8</td>
<td>248.2</td>
<td>26.3</td>
<td>53.8</td>
<td>-26.3</td>
<td>-0.1</td>
</tr>
<tr>
<td>$S_2$ (g)</td>
<td>64.1</td>
<td>128.6</td>
<td>228.2</td>
<td>34.1</td>
<td>4.7</td>
<td>-1.1</td>
<td>-2.6</td>
</tr>
<tr>
<td>$S_4$ (g)</td>
<td>128.3</td>
<td>135.6</td>
<td>293.6</td>
<td>72.7</td>
<td>18.1</td>
<td>-8.8</td>
<td>-10.1</td>
</tr>
<tr>
<td>$S_6$ (g)</td>
<td>192.4</td>
<td>101.3</td>
<td>357.8</td>
<td>130.2</td>
<td>0.8</td>
<td>2.6</td>
<td>-15.6</td>
</tr>
<tr>
<td>$S_8$ (g)</td>
<td>256.5</td>
<td>101.3</td>
<td>432.5</td>
<td>166.2</td>
<td>22.0</td>
<td>8.3</td>
<td>-15.1</td>
</tr>
<tr>
<td>$H_2O$ (l)</td>
<td>18.0</td>
<td>-285.8</td>
<td>70.0</td>
<td>186.9</td>
<td>-464.2</td>
<td>548.6</td>
<td>-19.6</td>
</tr>
<tr>
<td>$H_2O$ (g)</td>
<td>18.0</td>
<td>-241.8</td>
<td>188.8</td>
<td>28.4</td>
<td>12.5</td>
<td>0.4</td>
<td>1.3</td>
</tr>
<tr>
<td>$N_2$ (g)</td>
<td>28.0</td>
<td>0.0</td>
<td>191.6</td>
<td>27.2</td>
<td>2.5</td>
<td>3.2</td>
<td>0.8</td>
</tr>
<tr>
<td>$O_2$ (g)</td>
<td>32.0</td>
<td>0.0</td>
<td>205.1</td>
<td>22.3</td>
<td>20.5</td>
<td>-8.0</td>
<td>1.5</td>
</tr>
<tr>
<td>Component</td>
<td>Tb</td>
<td>Tm</td>
<td>AIT</td>
<td>ρ&lt;sub&gt;air&lt;/sub&gt;</td>
<td>ρ&lt;sub&gt;water&lt;/sub&gt;</td>
<td>MAC</td>
<td>LEL-UEL</td>
</tr>
<tr>
<td>-----------</td>
<td>----</td>
<td>----</td>
<td>-----</td>
<td>---------------</td>
<td>---------------</td>
<td>-----</td>
<td>---------</td>
</tr>
<tr>
<td></td>
<td>[°C]</td>
<td>[°C]</td>
<td>[°C]</td>
<td>[-]</td>
<td>[-]</td>
<td>[ppm]</td>
<td>[vol%]</td>
</tr>
<tr>
<td>S&lt;sub&gt;445,114,235&lt;/sub&gt;</td>
<td>445</td>
<td>114</td>
<td>235</td>
<td>-</td>
<td>-</td>
<td>2.07</td>
<td>-</td>
</tr>
<tr>
<td>H&lt;sub&gt;2&lt;/sub&gt;O</td>
<td>100</td>
<td>0</td>
<td>-</td>
<td>-</td>
<td>1.0</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CS&lt;sub&gt;2&lt;/sub&gt;</td>
<td>46</td>
<td>-112</td>
<td>100</td>
<td>2.6</td>
<td>1.3</td>
<td>20H</td>
<td>1.0-60</td>
</tr>
</tbody>
</table>

Table 3.3. Physical properties of the substances present in the designed process.
<table>
<thead>
<tr>
<th>Compound</th>
<th>Lower Limit</th>
<th>Upper Limit</th>
<th>Flash Point</th>
<th>Lower Flash</th>
<th>Upper Flash</th>
<th>Lower Explosion</th>
<th>Upper Explosion</th>
</tr>
</thead>
<tbody>
<tr>
<td>NO₂</td>
<td>21</td>
<td>-11</td>
<td>-</td>
<td>1.6</td>
<td>1.45</td>
<td>2</td>
<td>-</td>
</tr>
<tr>
<td>C₄H₁₀</td>
<td>-0.5</td>
<td>-138</td>
<td>365</td>
<td>2.01</td>
<td>0.58</td>
<td>600</td>
<td>1.3-8.5</td>
</tr>
<tr>
<td>SO₂</td>
<td>-10</td>
<td>-76</td>
<td>-</td>
<td>2.3</td>
<td>1.4</td>
<td>2</td>
<td>-</td>
</tr>
<tr>
<td>C₃H₈</td>
<td>-42</td>
<td>-187</td>
<td>470</td>
<td>1.6</td>
<td>0.5</td>
<td>-</td>
<td>1.7-9.5</td>
</tr>
<tr>
<td>COS</td>
<td>-50</td>
<td>-139</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>H₂S</td>
<td>-60</td>
<td>-86</td>
<td>260</td>
<td>1.2</td>
<td>0.8</td>
<td>10</td>
<td>4.0-46</td>
</tr>
<tr>
<td>CO₂</td>
<td>-79</td>
<td>-</td>
<td>-</td>
<td>1.5</td>
<td>0.8</td>
<td>5000</td>
<td>-</td>
</tr>
<tr>
<td>C₂H₆</td>
<td>-89</td>
<td>-183</td>
<td>515</td>
<td>1.04</td>
<td>0.4</td>
<td>-</td>
<td>2.7-12.5</td>
</tr>
<tr>
<td>NO</td>
<td>-152</td>
<td>-164</td>
<td>-</td>
<td>1.03</td>
<td>1.3</td>
<td>25</td>
<td>-</td>
</tr>
<tr>
<td>CH₄</td>
<td>-162</td>
<td>-182</td>
<td>537</td>
<td>0.6</td>
<td>-</td>
<td>-</td>
<td>5-16</td>
</tr>
<tr>
<td>O₂</td>
<td>-183</td>
<td>-218</td>
<td>-</td>
<td>1.1</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>N₂</td>
<td>-196</td>
<td>-</td>
<td>-</td>
<td>0.97</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>CO</td>
<td>-191</td>
<td>-205</td>
<td>605</td>
<td>0.97</td>
<td>-</td>
<td>25</td>
<td>11.0-75</td>
</tr>
<tr>
<td>H₂</td>
<td>-253</td>
<td>-259</td>
<td>-</td>
<td>0.07</td>
<td>-</td>
<td>-</td>
<td>4-76</td>
</tr>
</tbody>
</table>

* The explosion limits of sulfur in air are 35-1400 g/m³.
4 PROCESS STRUCTURE AND PROCESS FLOWSHEET

4.1 MOTIVATION OF PROCESS STRUCTURE

In order to make clear the reasons for choosing the final process structure the constraints and difficulties of the IFB NOXSO Unit and the Sulfur Recovery Unit will be described first. Then the solution for these problems and the final process structure will be described.

4.1.1 CONSTRAINTS TO THE IFB NOXSO UNIT PROCESS STRUCTURE

During simulation of the IFB NOXSO Unit it became clear that the IFB reactors and the gas streams through these reactors would become quite big. In order to reduce the costs, recycles are wanted and reactors should be as small as possible. A recycle over the adsorber however is not a good option. It would dilute the flue gas stream and therefore a bigger reactor would be needed. Also the heater cannot be equipped with a recycle stream. The reason is the concentration of NO\textsubscript{x} in the gas stream would become to high thus it becomes harder to remove the NO\textsubscript{x} from the sorbent because of equilibrium composition shifts.

The regenerator is fed with a nitrogen/natural gas stream. The reason for this is that the regeneration needs a reducing atmosphere. When using nitrogen and natural gas such an atmosphere is created. If only natural gas is used a lot of CO\textsubscript{2} would be produced in the reductors of the SRU. This CO\textsubscript{2} would be recycled and thus reduce the regenerating capabilities of the regenerator. Of course also hydrogen could be used and no CO\textsubscript{2} would be produced in the reductors. Natural gas however gives better results and is cheaper. The nitrogen stream is a big stream and surely has to be recycled.

Finally, the cooler. According to preliminary calculations the cooler would become the biggest reactor of all and would need the biggest gas stream. This IFB reactor must be equipped with a recycle stream.

4.1.2 CONSTRAINTS TO THE SULFUR RECOVERY UNIT PROCESS STRUCTURE

Process route 1 as described in §3.1, in which partial reduction of sulfur dioxide takes place followed by the catalytic Claus steps, was examined and rejected because the goal to recover 95% of the sulfur in the feed stream of the process could not be met. Major reason for the low sulfur recovery is the fact that a furnace is not part of this process route. This furnace would be responsible for the major part of the sulfur dioxide conversion.

It also became clear that water, present in the process stream after the sulfur dioxide reduction step, will lead to major problems in the Claus steps. As a result of the fact that the feed of the superclaus SRU contains a large amount of water, the equilibria in the Claus steps will be influenced unfavourably. The precise reason for this will follow in §4.3.3.3. Efforts to condense the water between the several process steps did not succeed as well.
Process units:

1. power station
2. adsorber
3. heater
4. regenerator
5. cooler
6. SO₂ reduction
7. CO₂ reduction
8. towers
9. Claus reactors
10. superclaus reactor
11. incinerator

Figure 4.1 Process scheme of the factory after literature research

* where is your adapted scheme?
* at what T, P levels? (per block)
Process route 2 as described in §3.1, in which complete reduction takes place followed by a complete superclaus plant, was also rejected because of a sulfur recovery which is too low in spite of the fact that here a furnace is present. Here also the same equilibrium problems occurred with water and carbon dioxide.

4.1.3 SOLUTIONS AND DESCRIPTION OF THE PROCESS STRUCTURE

The solution for the problems occurring due to the excess of water in the SRU is to build in a carbon dioxide reduction step and absorption/desorption tower unit after the sulfur dioxide reduction step. In this tower unit the water can be removed and so the SRU will be smaller and will have better results.

The reduction steps of sulfur dioxide and carbon dioxide are carried out with the use of hydrogen. This will be done, because otherwise the amount of produced carbon dioxide in the reduction step of sulfur dioxide would be too large when using for example methane instead of hydrogen.

For the fact that in the absorption tower containing diethanolamine (DEA) only hydrogen sulfide and carbon dioxide will be absorbed, the sulfur reduction step will have to be as complete as possible. In fact process route 2 of §3.1 will be followed in an adjusted way (Figure 3.1, route 3).

Now a gas stream containing the nitrogen, some carbon dioxide and the by carbon dioxide reduction formed methane can be sent back to the regenerator. This process structure, route 3 (Figure 4.1), will be followed in this PDA.

The final process structure can be described as follows. The developed plant consists of an IFB NOXSO Unit, a 'Connect Unit' and a Sulfur Recovery Unit. This 'Connect Unit' connects the IFB NOXSO Unit and the SRU.

The IFB NOXSO Unit consists of four IFB reactors. These are an adsorber, a heater, a regenerator and a cooler. In the adsorber the flue gas from the 150 MWe electrical power plant is cleaned. From the heater the NOx is sent back to the electrical power plant and from the regenerator the SO2 and H2S are sent to the 'Connect Unit'.

The 'Connect Unit' consists of the reduction step of sulfur dioxide to hydrogen sulfide, the reduction step of carbon dioxide to methane and an absorber/stripper tower unit. This part of the plant connects the IFB NOXSO Unit and the superclaus SRU in which the sulfur is recovered.

In this configuration the absorber/stripper tower combination is the critical step. In this unit hydrogen sulfide passes almost completely and carbon dioxide passes only partially to the superclaus SRU. The rest of the process stream entering the towers is recycled to the IFB NOXSO Unit. Part of the gas stream of the recycle stream has to be purged.

The carbon dioxide and hydrogen sulfide stream is fed to a superclaus sulfur recovery unit containing a furnace, two catalytic Claus reactors and a superclaus reactor. In the superclaus reactor this stream is selectively oxidized by air. To this reactor the recycle purge is added for two reasons. The major reason is the fact that concentration of hydrogen sulfide in the feed stream of the superclaus reactor should not be too high. The purge stream dilutes the feed stream so the volumetric concentration of hydrogen sulfide is of the order 1 - 2 [m3 H2S/m3 stream].

After the Claus furnace, the two catalytic Claus reactors and the superclaus reactor the produced sulfur (S) is separated from the process stream and led to a sulfur storage tank.
Figure 4.2 NOXSO desulfurization process applied in IFB system
Finally the process stream is fed to an incinerator in which all the remaining components are oxidized by air. It is of upmost importance that the remaining hydrogen sulfide is oxidized to sulfur dioxide because of environmental regulations.

4.2 DESCRIPTION OF PROCESS UNITS

The process flowsheet (Appendix 8) will be followed in discussing the various units of the designed plant. The occurring reactions and the thermodynamics for each process unit will be treated in §4.3.

4.2.1 IFB NOXSO UNIT

The main reason for choosing the Interconnected Fluidized Bed system is the low rate of catalyst attrition. In this system the sorbent is not transported between the fluidized bed reactors through pipes but through other fluidized beds. These are the transport beds and are called the 'dense beds' because these beds are only just fluidized. The other beds, where the reactions take place, are called the 'lean beds'. Particles flow from the lean bed over a weir into the dense bed. Then the particles flow down through the dense bed to an orifice which connects this dense bed with the next lean bed. This way the sorbent particles are transported from one lean bed to another. Figure 4.2 is an example of how these systems can be constructed.

Where possible the gas streams needed to fluidize the beds are chosen to be air streams. This is done because air is cheap. The pressure of these streams will be atmospheric because the flue gas is available at this kind of pressure. Another reason is reduction of the compressor costs; the power plant manager will not be pleased when a considerable amount of the produced electricity will be used for the cleaning of the flue gas stream of his plant.

4.2.1.1 ADSORBER

In the lean bed of the adsorber (R11) the flue gas is used to fluidize the bed. In this bed the requested amount of NOx and SOx is removed from the flue gas. This is done by adsorption of these components on a sorbent.

This sorbent consists of Na2O sites on γ-alumina. The properties of this sorbent are presented in Appendix 9. In this reactor the needed sorbent stream can be determined in order to clean the flue gas stream.

The flue gas stream enters the lean bed at a temperature of about 120 °C and this is also the temperature at which the adsorption works best [17 and 19]. The pressure is about 2 bar. The overall adsorption described in §4.3.1.1 is exothermic. The temperature can be held at about 120 °C by spraying water in the lean bed. This water will vaporize and thus cool the fluidized bed.

The dense bed (or transport) bed of the adsorber (R12) is kept at minimum fluidization by air. This air stream is chosen to be at the same conditions as the flue gas stream. The temperature is 120 °C and the pressure is about 2 bar. This way the process conditions of the lean and the dense bed at the top of the weir do not differ too much and the process conditions will remain most optimal. Otherwise there might be some desorption because of a deviation of the optimal process conditions.
4.2.1.2 HEATER

In the lean bed of the heater (R18) the NO\textsubscript{x} is removed from the sorbent. This bed is kept fluidized by an air stream of 1000 °C and 2 bar. The heater (and the cooler) can be configured in several ways. The way this temperature and configuration are obtained, is explained in the calculations in §5.2.1.3.

The dense bed (R19) is used as a stripping bed where the last traces of NO\textsubscript{x} are removed. This is done with steam at 680 °C and 2 bar. Because of safety reasons the temperature was chosen this high. These reasons are described in §9.1.

4.2.1.3 REGENERATOR

In the lean bed of the regenerator (R23) the sulfur containing compounds are removed from the sorbent. This is done using a nitrogen/natural gas stream at 620 °C and 2 bar. These are the optimal process conditions according to Ma [17].

A nitrogen/natural gas stream is chosen because for the regeneration a reducing atmosphere is needed. When using nitrogen and natural gas such an atmosphere is created. When only using natural gas a lot of CO\textsubscript{2} would be produced in the reductors of the 'Connect Unit'. This CO\textsubscript{2} would be recycled and thus reducing the regenerating capabilities of the regenerator. Of course also hydrogen could be used and no CO\textsubscript{2} would be produced in the reductors. Natural gas however gives the better results and is cheaper [17].

The dense bed (R24) is used as a stripping bed in which the last traces of sulfur containing compounds are removed. This is done with steam at 620 °C and 2 bar.

4.2.1.4 COOLER

In the lean bed of the cooler (R28) the sorbent and the small particles that are formed by attrition in the IFB system are blown out. The cooler can be configured in several ways. The chosen configuration is explained in the calculations in §5.2.1.2. For the cooling part an air stream of 25 °C and 2 bar is used. This way the temperature difference will be maximal and thus the driving force for heat transfer is maximal.

For the removal of the small particles that are due to attrition an air stream of 120 °C and 2 bar is used. This temperature is chosen because this removal is done after the particles are cooled down to 120 °C. The particles are removed in this part of the IFB NO\textsubscript{X}SO Unit because in the cooler the particles contain the smallest amount of sulfur containing compounds. Therefore the loss of sulfur will be small.

The dense bed (R29) is used as a transport bed, as a sorbent flow regulation bed and for adding fresh sorbent particles to the IFB system. For the same reason as the particle removal an air stream of 120 °C and 2 bar is used.

The air used for the cooler is prepared using a compressor and a heat exchanger. At the process conditions however water will condensate. Therefore the two liquid/vapour separators (V26 and V31) are used to remove the water. Then the air can be used for the cooler.
4.2.2 CONNECT UNIT

4.2.2.1 REDUCTION STEP OF SULFUR DIOXIDE TO HYDROGEN SULFIDE

The reduction of sulfur dioxide (R32) with hydrogen takes place over an activated bauxite catalyst [2].

Table 4.1. Approximate composition of activated bauxite catalyst

<table>
<thead>
<tr>
<th>Component</th>
<th>Mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>[•]</td>
<td>[wt%]</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>88</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>2.5</td>
</tr>
<tr>
<td>TiO₂</td>
<td>3.0</td>
</tr>
<tr>
<td>SiO₂</td>
<td>6.5</td>
</tr>
</tbody>
</table>

To get highest possible conversion of sulfur dioxide to hydrogen sulfide the temperature of the reaction should be between 380 °C and 395 °C. The conversion of sulfur dioxide is then approximately 98%. The pressure during this reduction, which is exothermal, will be atmospheric.

Most important by-product in this reduction step will be sulfur. Sulfur here is considered as a by-product because first the sulfur dioxide has to be converted into hydrogen sulfide in order to separate the sulfur containing compounds as much as possible from the other components of the process stream. It is also not possible to produce a considerable amount of sulfur and a near to complete conversion of sulfur dioxide to hydrogen sulfide. The precise reason for this separation of hydrogen sulfide of the process stream was mentioned in §4.1.2.

Is sulphur in the vapour phase?
Does the sulphur affect downstream catalyst (beds)?
Stream table does not show any sulphur
4.2.2.2 REDUCTION STEP OF CARBON DIOXIDE TO METHANE

The reduction of carbon dioxide (R44) with hydrogen is carried out over a nickel magnesium oxide catalyst on a γ-alumina support [5]. Sulfur however will poison nickel (Ni) by chemisorption. Thus the catalyst will slowly deactivate. An alternate for Ni in the catalyst could be molybdenum (Mo) or wolframe (W). However the activity of the catalyst would be much lower than the catalyst containing Ni. This catalyst can be used because of the fact that only small amounts of sulfur will be present here. The optimal reaction temperature is 360 °C. The reduction is carried out with an absolute pressure of 25 bar.

Most important by-product of this reaction is water.

The reduction of carbon dioxide is very exothermic ($\Delta H_{r,298} = -164,91$ kJ/mol), therefore the major problem with this step is the discharge of the reaction heat. The used packed bed reactor is well isolated so the reaction is adiabatic.

4.2.2.3 ABSORPTION/STRIPPER TOWER UNIT

In this unit hydrogen sulfide will be absorbed. In addition to this, carbon dioxide is absorbed as well. Only hydrogen sulfide and carbon dioxide will flow to the superclaus SRU of the designed plant.

The absorbent in the tower unit is a diluted diethanolamine solution (DEA) [6]. Another option for the used absorbent could have been monoethanolamine (MEA). MEA is mostly used for this purpose. However in this process also carbonyl sulfide (COS) is present; in presence of COS, MEA is no longer regenerable and therefore MEA is not the appropriate absorbent. According to Kohl [6] DEA is the best alternate for MEA.

4.2.2.3.1 ABSORPTION TOWER

In the absorption tower (T49) hydrogen sulfide and carbon dioxide is absorbed by a diluted DEA solution. This loaded DEA solution (= rich solution) leaves the tower over the bottom and flows to the stripper tower. The rest of the process stream is recycled over the top of the absorber tower to the regenerator of the IFB NOXSO Unit. The packing of the tower consists of stoneware raschig rings. A packed column is used instead of a tray column because in a tray column foam formation will occur. This will result in a less effective absorption. Besides a packed column has a bigger carbon dioxide removal efficiency.

The efficiency for the absorption is 90.8% for hydrogen sulfide and 52.2% for carbon dioxide. The operation temperature in this tower is 40 °C; the working pressure is 25 bar.

4.2.2.3.2 STRIPPER TOWER

In the stripper tower (T52) the diluted DEA solution (= rich solution) loaded with sulfur dioxide and carbon dioxide is stripped by steam. The stripped carbon dioxide and hydrogen sulfide together with steam then leave over the tower top and is passed through a flash vessel in which the steam is condensed.
Of course the steam rate needed for stripping depends on the solution rate that
is pumped between the towers. The stripped diluted DEA solution (= lean solution) is
then recycled to the absorption tower over the bottom of the stripper tower.

The stripper tower is a tray column. Above the feed point two to six trays are
present; below the feed point twelve to twenty trays are installed. Because of the fact
that DEA is the trays above the feed point will be needed above to recover the amine
vapours and to remove entrained amine droplets that occurred due to foaming.

The height of the stripper tower is usually determined in practice on the base
of experimental work. The operational temperature and absolute pressure at the top
of the tower are 97.9 °C and 1.38 bar. The operational temperature and absolute
pressure at the bottom of the tower are 115.7 °C and 1.65 bar.

4.2.3 THE SUPERCLAUS SULFUR RECOVERY UNIT

The superclaus SRU consists of a furnace, two catalytic Claus reactors, a
superclaus reactor and an incinerator. In this configuration also four gas-liquid
separators and heaters are present.

The superclaus process is operated at atmospheric pressure. The reactions in
the superclaus SRU are exothermal. The superclaus SRU can is capable of a sulfur
yield of over 99.9%.

4.2.3.1 THE CLAUS FURNACE AND THE WASTE HEAT BOILER

For a superclaus plant the furnace (F64) is a crucial unit in respect to the sulfur
recovery. In this unit a sulfur yield just less than 70% can be obtained [1]. It is of
upmost importance to regulate the air supply in order to obtain a H2S to SO2 outgoing
concentration ratio of 2. This is the required concentration ratio for the catalytic Claus
reaction. Due to the kinetically and thermodynamically favourable equilibrium
composition in the furnace in regard to hydrogen sulfide conversion (§4.3.3.1) a
catalyst is not needed.

In this process the most important secondary reactions are those which are
responsible for the formation of carbon sulfide (CS2) and carbonyl sulfide (COS). The
higher the hydrocarbon content in the feed stream of the furnace the more CS2 and
COS will be produced.

During combustion the temperature is between 925 °C and 1600 °C. Beyond
these temperatures the flame gets unstable. Above 1600 °C the material limits are
crossed.

The furnace is isothermally operated and combined with a waste heat boiler.
By cooling the hot gases (1027 °C) in the combined furnace/waste heat boiler high
pressure steam (40 bar) is produced.

4.2.3.2 THE CONDENSORS/VAPOUR-LIQUID SEPARATORS

In the condensers (H58/H60/H65, H69, H73, H78) the produced sulfur in the
furnace, the two catalytic Claus reactors and the superclaus reactor is condensed by
cooling (further detail on cooling §5.4.2). The efficiency of these condensors is of
course depending on the operating temperature. The operating temperature thus
should be below the dewpoint of sulfur.
Figure 4.3: Theoretical conversion of $\text{H}_2\text{S}$ to vapor sulfur.
In the vapour-liquid separators the condensed sulfur is separated from the rest of the process stream and passed through a seal pit to a sulfur storage tank. A major problem with the condensers is the formation of sulfur mist. This mist has to be removed in order to prevent loss in efficiency of sulfur formation in the catalytic beds. This problem can be overcome by de-misters [7].

4.2.3.3 THE (PRE)HEATERS

The process stream entering the catalyzed reactors of the superclaus SRU is preheated (H16, H17, H10) in order to reach the appropriate temperature for entering the catalytic reactors; however another important reason this preheating should take place is the fact that otherwise also a small amount of liquid sulfur will enter the catalytic beds. The liquid sulfur will plug (deactivate) the catalyst and thus reduce the conversion to sulfur.

Preheating of the feed of the catalytic reactors can be done in several ways [7]:

1. Direct mixing
   A hot gas bypass is used to heat the process stream entering the catalytic reactor. The process stream entering one of the catalytic reactors is mixed with a part of the gas stream coming out of a preceding reactor of the superclaus SRU. Here the costs of the heating device will be low of course; however the sulfur recovery efficiency will be reduced significantly.

2. Fired heaters
   The heating of the process stream is done by burning fuel (natural gas) in a furnace. It can also be done by burning a small amount of the process gas. Usually also a small part of the hot stream coming out of the reactor before the sulfur condenser is mixed with the process stream to be heated.
   In case of a low air to acid gas ratio SO₃ will be formed. This will deactivate the catalyst in the catalytic bed.

3. Indirect heating.
   Here gas to gas heat exchange is carried out. The gas stream by which the process stream is heated consists of oil, steam or the outlet of another reactor of the process. This heating procedure is commonly used in industrial processes because it will result in the highest sulfur recovery efficiency.

4.2.3.4 THE CATALYTIC CLAUS REACTORS

The catalytic Claus reactors (R68, R72) consist of a packed bed; the reactor is well isolated and therefore operates adiabatically.

As mentioned earlier (§4.2.3.1) the H₂S to SO₂ ratio of the feed stream must be 2 in order to obtain the optimal sulfur yield in these steps. The operating temperatures here are much lower than for the Claus furnace (see Figure 4.3). The lowest temperature possible for this reaction step is determined by the dewpoint of sulfur. Condensation of sulfur should be avoided of course. For thermodynamic reasons the catalytic unit should be operated at as low temperature as possible above the dewpoint of sulfur provided the rate of reaction is fast enough. Usually the catalytic Claus reactors are operated at 350 - 390 °C. At these temperatures the best catalyst for this reaction is the Kaiser S-501 catalyst (surface area: 270 m²/g) [1]. This catalyst converts almost 100% of the produced COS; the conversion of CS₂ is slightly lower

*How to control H₂S/ SO₂ ratio
No independent SO₂ feed to match H₂S.*
Figure 4.4: The performance of sodium promoted 5 wt% Fe₂O₃ on silica catalyst. -○- H₂S conversion, -●- selectivity to sulfur, compared to the standard catalyst: -□- H₂S conversion, -■- selectivity to sulfur.
than other commercially used Claus catalysts like activated bauxite. The concentration of produced CS$_2$ and COS must be kept as low as possible because these components cause deactivation of the catalyst. CO$_2$ is also a carbon containing compound but this is not a potential source of catalyst deactivation. However carbon dioxide can be a precursor of carbon sulfide.

To obtain an optimum yield of sulfur the second Claus converter should operate at lower temperature than the first one. This way the Claus equilibrium will be favourably changed towards sulfur.

The Kaiser S-501 catalyst is a sulfated activated alumina catalyst. The sulfated catalyst has a slightly lower efficiency of converting CS$_2$ however on a sulfated catalyst less SO$_3$ will adsorb on the catalyst surface comparing to other commercial Claus catalysts. SO$_3$ will cause catalyst deactivation as well. Claus catalyst deactivation is caused by [1]:

- deposition of coal on the catalyst surface
- sulfate adsorption on the catalyst surface and
- thermal aging.

4.2.3.5 THE SUPERCLAUS REACTOR

The superclaus reactor (R77) consists of a well isolated packed bed reactor. So this unit will operate adiabatically.

In the superclaus unit sulfur is produced by selective oxidation of H$_2$S over a sodium promoted 5wt% Fe$_2$O$_3$ on silica [3]. The optimum operating temperature is 240 °C. The hydrogen sulfide conversion will be 95% and the sulfur yield will be 96%. The volumetric hydrogen sulfide concentration of the feed of the superclaus reactor has to be within the range of 1 - 2 vol%.

The selectivity to sulfur formation of the used superclaus is high over a wide range of temperatures (see Figure 4.4). This property of the sodium promoted iron oxide catalyst on silica support combined with its high conversion of hydrogen sulfide makes it a better catalyst for the superclaus reaction compared to other commercial superclaus catalysts like a FeSO$_4$ on a silica support catalyst or a Fe$_2$O$_3$/Cr$_2$O$_3$ catalyst on an α-alumina support.

The superclaus catalyst must be a wide pore catalyst and have a low surface area. The first restriction is related to the fact that water condensation will occur in narrow pore catalysts. Water is a good Claus catalyst; water causes the reverse Claus reaction (see also §4.3.3.4) to take place. This way the hydrogen sulfide conversion will reduce. The reverse Claus reaction is also prevented by the sodium promoter of the catalyst. The second restriction (low surface area of the catalyst (7 m$^2$/g)) must be obeyed because this way a low sulfur concentration will occur at the catalyst surface area. This will result in low sulfur poisoning of the catalyst. Sulfur poisoning is a function of the surface concentration of sulfur, temperature and structure of catalyst.

Of course also thermal aging is here a source of deactivation of the catalyst.

4.2.3.6 THE INCINERATOR/STACK

In the incinerator (F86) the remaining hydrogen sulfide is oxidized to sulfur dioxide. Sulfur dioxide is less harmful (hazardous) for the environment than hydrogen sulfide because it is less corrosive. Also CS$_2$ and COS will be oxidized in this furnace.

In this unit no catalyst will be used. Furthermore the unit is operated at
temperatures of 537 - 816 °C and with an oxygen excess of 20 - 25 vol% [8].

The unit is operated adiabatically. The hot outgoing gas stream is heat exchanged with other process gas streams and finally low pressure steam (3 bar) is produced.

The height of the stack (M89) is depending on the amount/concentration of SO₂ in the gas stream. Usually the height of the stack will be governed by local pollution regulations. A save height for the discharge of SO₂ is 30 m [8].

4.3 PROCESS CONDITIONS, REACTIONS AND KINETICS

In this chapter the reactions occurring and the kinetics of these reactions will be discussed. Also the operational conditions will be mentioned. In addition to the part of the Connect Unit and the Sulfur Recovery Unit the thermodynamics of equilibria and the several sulfur species are considered. It is assumed that in only the equipment that is mentioned in the following text reactions will occur. In all the other equipment it is assumed that no reactions will take place. In practice this will not be the case; however the significance of these reactions can probably be neglected.

4.3.1 IFB NOXSO UNIT

The places in the IFB NOXSO Unit where reactions occur are the adsorber, the heater and the regenerator. The reactions and the kinetics in these reactors will be discussed now.

4.3.1.1 ADSORBER

In the adsorber SO₂ and NOₓ is removed from a flue gas stream by adsorption on a sorbent. The most important reactions that occur in the adsorber are according to Ma[17]:

\[
SO_2 + Na_2O \rightleftharpoons k_1 \cdot k_1' \rightarrow Na_2OSO_2 \quad (4.1)
\]

\[
Na_2OSO_2 + 2 NO_x \rightleftharpoons k_2 \cdot k_2' \rightarrow (NO_x)_2Na_2O + SO_2 \quad (4.2)
\]

\[
Na_2OSO_2 \rightarrow k_3 \rightarrow Na_2OSO_3 \quad (4.3)
\]

In the same article of Ma [17] the reaction constants of these reactions are mentioned:

\[
K_1 = \frac{k_1}{k_1'} = 2000 \frac{1}{atm} \quad (4.4)
\]
\[ K_2 = \frac{k_2}{k'_2} = 1.2 \frac{1}{\text{atm}} \quad (4.5) \]

\[ k_2 = 5.8 \frac{1}{s \text{ atm}^2} \quad (4.6) \]

\[ k_3 = 0.0012 \frac{1}{s} \quad (4.7) \]

Now with the model that NOXSO provides in [17] the adsorber can be simulated. The temperature used will be 120 °C and the pressure will be 2 bar. At these conditions the adsorption works best.

4.3.1.2 HEATER

In the heater the sorbent is heated to the right temperature for the regeneration step. During the heating according to Ma [17] all the NO\textsubscript{x} is removed from the sorbent. No reactions for this step have been found. This heater will be fed with a air stream of 1000 °C and 2 bar.

4.3.1.3 REGENERATOR

In the regenerator the SO\textsubscript{2} and SO\textsubscript{3} is removed from the Na\textsubscript{2}O sites of the sorbent. This is done by using natural gas. The reactions that occur with methane according to Yeh [18] are:

\[
\begin{align*}
4 \text{Na}_2\text{OSO}_3 + \text{CH}_4 & \rightarrow 4 \text{Na}_2\text{OSO}_2 + 2 \text{H}_2\text{O} \\
4 \text{Na}_2\text{OSO}_2 + 3 \text{CH}_4 & \rightarrow 4 \text{Na}_2\text{S} + 3 \text{CO}_2 + 6 \text{H}_2\text{O} \\
\text{Al}_2\text{O}_3 + \text{Na}_2\text{OSO}_2 & \rightarrow \text{Na}_2\text{OAl}_2\text{O}_3 + \text{SO}_2 \\
\text{Al}_2\text{O}_3 + \text{Na}_2\text{S} + \text{H}_2\text{O} & \rightarrow \text{Na}_2\text{OAl}_2\text{O}_3 + \text{H}_2\text{S}
\end{align*}
\]

(4.8) (4.9) (4.10) (4.11)

Yeh did not find any Na\textsubscript{2}S in his studies but thought it to be the most likely intermediate.

With the facts that there will be no nett Na\textsubscript{2}S production, that according to Leonard [19] the produced SO\textsubscript{2}/H\textsubscript{2}S ratio is 2 and with the model for the regeneration described by Ma [17] the regenerator can be modelled. This will be done with a nitrogen/natural gas stream at 620°C and 2 bar.

I do not understand this.
4.3.2 CONNECT UNIT

4.3.2.1 THE REDUCTION STEP OF SULFUR DIOXIDE WITH HYDROGEN

In this reactor the sulfur dioxide present in the process stream will be reduced nearly to completion with hydrogen.

The following reactions occur [2]:

\[
\begin{align*}
2 \text{SO}_2 + 4 \text{H}_2 & \iff \text{S}_2 + 4 \text{H}_2\text{O} \\
2 \text{H}_2 + \text{S}_2 & \iff 2 \text{H}_2\text{S} \\
2 \text{S}_2 & \iff \text{S}_4 \\
3 \text{S}_2 & \iff \text{S}_6 \\
4 \text{S}_2 & \iff \text{S}_8 \\
2 \text{SO}_2 + \text{CH}_4 & \iff 2 \text{H}_2\text{O} + \text{S}_2 + \text{CO}_2
\end{align*}
\]

The hydrogen to sulfur dioxide ratio here is just slightly bigger than 3 (3.01), therefore the formation of hydrogen sulfide is favoured [2]. If this ratio would have been smaller than 2, the formation of sulfur would have been favoured.

The operating temperature is 384.1 °C; the absolute pressure is 1.93 bar.

4.3.2.2 THE REDUCTION STEP OF CARBON DIOXIDE WITH HYDROGEN

Conversions of carbon dioxide close to unity can be obtained with subjoined equilibrium reactions by applying the right process conditions. The catalyst being used is the γ-alumina supported Ni-MgO catalyst. The following reactions occur [5]:

\[
\begin{align*}
\text{CO} + 3 \text{H}_2 & \iff \text{CH}_4 + \text{H}_2\text{O} \\
2 \text{CO} + 2 \text{H}_2 & \iff \text{CH}_4 + \text{CO}_2 \\
\text{CO}_2 + 4 \text{H}_2 & \iff \text{CH}_4 + 2 \text{H}_2\text{O} \\
\text{CO} + \text{H}_2\text{O} & \iff \text{CO}_2 + \text{H}_2 \\
2 \text{CO} & \iff \text{CO}_2 + \text{C} \\
\text{CH}_4 & \iff 2 \text{H}_2 + \text{C} \\
\text{S}_2 + 2 \text{H}_2 & \iff 2 \text{H}_2\text{S}
\end{align*}
\]

The reaction marked with \( . \) can be obtained by using the reactions which are shown underneath:

\[
\begin{align*}
\text{CO}_2 + \text{H}_2 & \iff \text{CO} + \text{H}_2\text{O} \\
\text{CO} + 3 \text{H}_2 & \iff \text{CH}_4 + \text{H}_2\text{O} \\
\text{CO}_2 + 4 \text{H}_2 & \iff \text{CH}_4 + 2 \text{H}_2\text{O}
\end{align*}
\]

Reactions (4.20.1) and (4.20.2) are the main reactions of this reduction step. The temperature and pressure at which the carbon dioxide reduction to methane is processed are respectively 359.7 °C and 25.6 bar.
4.3.2.3 THE ABSORPTION OF CARBON DIOXIDE AND SULFUR DIOXIDE

The reaction equations describing the chemistry of the simultaneous absorption of carbon dioxide and sulfur dioxide in an aqueous solution of diethanolamine (DEA) are presented underneath [11]:

\[
\begin{align*}
\text{CO}_2 + \text{H}_2\text{O} + \text{C}_4\text{H}_{13}\text{O}_2\text{N} & \iff \text{HCO}_3^- + \text{C}_4\text{H}_{13}\text{O}_2\text{NH}^+ \quad (4.25) \\
\text{CO}_2 + 2 \text{C}_4\text{H}_{13}\text{O}_2\text{NH}^- & \iff \text{C}_4\text{H}_{13}\text{O}_2\text{NH}_2^+ + \text{C}_4\text{H}_{13}\text{O}_2\text{NCO}_3^- (4.26) \\
\text{CO}_2 + \text{OH}^- & \iff \text{HCO}_3^- \quad (4.27) \\
\text{HCO}_3^- + \text{OH}^- & \iff \text{CO}_3^{2-} + \text{H}_2\text{O} \quad (4.28) \\
\text{H}_2\text{S} + \text{C}_4\text{H}_{13}\text{O}_2\text{N} & \iff \text{C}_4\text{H}_{13}\text{O}_2\text{NH}^+ + \text{HS}^- \quad (4.29) \\
\text{H}_2\text{S} + \text{C}_4\text{H}_{13}\text{O}_2\text{NH}^+ & \iff \text{C}_4\text{H}_{13}\text{O}_2\text{NH}_2^+ + \text{HS}^- \quad (4.30) \\
\text{H}_2\text{O}^+ + \text{OH}^- & \iff 2\text{H}_2\text{O} \quad (4.31) \\
\text{HS}^- + \text{OH}^- & \iff \text{S}^{2-} + \text{H}_2\text{O} \quad (4.32)
\end{align*}
\]

By combination of reactions (4.33), (4.34) and (4.35) reaction numbers (4.29) and (4.30) can be obtained.

\[
\begin{align*}
\text{H}_2\text{S} + \text{OH}^- & \iff \text{HS}^- + \text{H}_2\text{O} \quad (4.33) \\
\text{C}_4\text{H}_{13}\text{O}_2\text{NH}^- + \text{OH}^- & \iff \text{C}_4\text{H}_{13}\text{O}_2\text{N} + \text{H}_2\text{O} \quad (4.34) \\
\text{C}_4\text{H}_{13}\text{O}_2\text{NH}^+ + \text{OH}^- & \iff \text{C}_4\text{H}_{13}\text{O}_2\text{NH}_2^+ + \text{H}_2\text{O} \quad (4.35)
\end{align*}
\]

The reaction rate of carbon dioxide for the reaction with the secondary amine diethanol amine is much lower than that with hydrogen sulfide. The reaction mechanism for absorption can be described using Higbie's theory. Considering the assumptions made in this PDA, further discussion of this mechanism is beyond the scope of the PDA.

The absorber tower is operated at 40 °C and 25 bar.

In the stripping tower the absorbed substances hydrogen sulfide and carbon dioxide is stripped from the aqueous solution of DEA. This is done by operating the tower at higher temperatures and lower pressure. This way the inverse reactions will occur.

The temperature and pressure at the top of the stripper tower are respectively 97.8 °C and 1.38 bar; at the bottom this is 115.6 °C and 1.65 bar respectively. The used solution is a 35 vol% DEA solution.

The flash vessel at the top of the stripper tower is operated at 50 °C and 1.3 bar.

4.3.2.4 KINETICS

The kinetics of the catalytic reduction of sulfur dioxide with hydrogen are known and presented by Murdock [2]. In this article it is also stated that it is thermodynamically possible to obtain essentially complete reduction of sulfur dioxide with the activated bauxite catalyst used. This is the major reason for modelling this reduction step with an equilibrium calculation. The equilibrium is shifted as much as possible to the right hand side by adjusting the hydrogen supply to the reactor for the effect wanted.
THEORETICAL EQUILIBRIUM CONVERSION OF HYDROGEN SULFIDE TO VAPOR SULFUR BY SELECTIVE OXIDATION WITH THE STOICHIOMETRIC AIR ACCORDING TO THE OVERALL EQUATION $2\text{H}_2\text{S} + \text{O}_2 = 2\text{H}_2\text{O} + 2/\text{e} \text{S}_\text{e}$.

Figure 4.5: Theoretical equilibrium conversion of hydrogen sulfide to vapor sulfur by selective oxidation with stoichiometric air according to the over-all reaction $2\text{H}_2\text{S} + \text{O}_2 = 2\text{H}_2\text{O} + 2/\text{e} \text{S}_\text{e}$. 
The reduction step of carbon dioxide with hydrogen to methane is also modelled using equilibrium calculations, because only the reaction rate of the most important catalyzed reaction (4.18) was known [5]. In this case it was thus not very realistic to simulate this reaction step using the kinetics of only one reaction, while several reactions took place. Furthermore it is stated by Biendarra [5] that the reduction could be simulated assuming thermodynamical equilibria. The catalyst used in this process is the γ-alumina supported Ni-MgO catalyst as mentioned earlier in this text (§4.2.2.2).

4.3.3 SUPERCLAUS SULFUR RECOVERY UNIT

4.3.3.1 THE FURNACE OF THE CLAUS SECTION

In the furnace a lot of reactions take place. Here we only consider the most significant reactions [10].

The occurring reactions are:

\[
\begin{align*}
2 \text{H}_2\text{S} + 3 \text{O}_2 & \leftrightarrow 2 \text{H}_2\text{O} + 2 \text{SO}_2 \\
4 \text{H}_2\text{S} + 2 \text{SO}_2 & \leftrightarrow 4 \text{H}_2\text{O} + 3 \text{S}_2 \\
\text{S}_2 + 2 \text{O}_2 & \leftrightarrow 2 \text{SO}_2 \\
2 \text{S}_2 & \leftrightarrow \text{S}_4 \\
3 \text{S}_2 & \leftrightarrow \text{S}_6 \\
4 \text{S}_2 & \leftrightarrow \text{S}_8 \\
2 \text{H}_2\text{S} + \text{O}_2 & \leftrightarrow 2 \text{H}_2\text{O} + \text{S}_2 \\
\text{CO}_2 + 2 \text{H}_2\text{S} & \leftrightarrow \text{CS}_2 + 2 \text{H}_2\text{O} \\
2 \text{CO}_2 & \leftrightarrow 2 \text{CO} + \text{O}_2 \\
\text{CO}_2 + \text{H}_2\text{S} & \leftrightarrow \text{COS} + \text{H}_2\text{O} \\
2 \text{H}_2\text{O} + \text{H}_2\text{S} & \leftrightarrow 3 \text{H}_2 + \text{SO}_2 \\
\text{S}_2 + 2 \text{H}_2 & \leftrightarrow 2 \text{H}_2\text{S}
\end{align*}
\]

For the Claus reaction (*) two temperature regions are available in which high hydrogen sulfide conversion can be obtained (see Figure 4.5) [9]. These two regions are the thermal and the catalytic region. The furnace is operated in the thermal region, therefore a catalyst is not needed. The operating temperature used is 1026.9 °C. The pressure is 1.9 bar.

4.3.3.2 THE CONDENSORS

Simultaneously with the chemical equilibrium reactions between the several sulfur species also a physical process takes place. This is the condensation of \( S_g \), reaction (4.51). The physical reaction is however included in the following reaction scheme.

\[
\begin{align*}
2 \text{S}_2 & \leftrightarrow \text{S}_4 \\
3 \text{S}_2 & \leftrightarrow \text{S}_6 \\
4 \text{S}_2 & \leftrightarrow \text{S}_8 \\
\text{S}_6 \text{(g)} & \leftrightarrow \text{S}_8 \text{(l)}
\end{align*}
\]

The operating temperature of the sulfur condensers is 154.3 °C according to the NOXSO design.
4.3.3.3 THE CATALYTIC CLAUS REACTORS

The subjoined catalyzed reactions [9] are catalysed by the Kaiser S-501 catalyst described above. To obtain high conversions, the temperature has to be kept low. So this unit operates in the catalytic region (see Figure 4.5). Due to the catalyst also the hydrolysis of carbonyl sulfide and carbon sulfide takes place.

\[
\begin{align*}
4 \text{H}_2\text{S} + 2 \text{SO}_2 & \rightleftharpoons 3 \text{S}_2 + 4 \text{H}_2\text{O} \quad (4.52') \\
4 \text{COS} + 2 \text{SO}_2 & \rightleftharpoons 3 \text{S}_2 + 4 \text{CO}_2 \quad (4.53) \\
\text{COS} + \text{H}_2\text{O} & \rightleftharpoons \text{CO}_2 + \text{H}_2\text{S} \quad (4.54) \\
\text{CS}_2 + 2 \text{H}_2\text{O} & \rightleftharpoons \text{CO}_2 + 2 \text{H}_2\text{S} \quad (4.55) \\
2 \text{S}_2 & \rightleftharpoons \text{S}_4 \quad (4.56) \\
3 \text{S}_2 & \rightleftharpoons \text{S}_6 \quad (4.57) \\
4 \text{S}_2 & \rightleftharpoons \text{S}_8 \quad (4.58)
\end{align*}
\]

The equilibrium of the Claus reaction (*) will not be at the sulfur side if the reacting stream contains a large amount of water. If a large concentration of water is present the equilibrium will shift towards the hydrogen sulfide side and less sulfur will be produced.

In the first Claus converter the temperature is 389.8 °C and the pressure is 1.84 bar. In the second Claus converter the process conditions are 374.4 °C and 1.65 bar.

4.3.3.4 THE SUPERCLAUS REACTOR

The reactions in the superclaus reactor are given below [3]. The catalyzed and most important reaction is reaction (4.59).

\[
\begin{align*}
2 \text{H}_2\text{S} + \text{O}_2 & \rightleftharpoons \text{S}_2 + 2 \text{H}_2\text{O} \quad (4.59) \\
2 \text{H}_2\text{S} + 3 \text{O}_2 & \rightleftharpoons 2 \text{SO}_2 + 2 \text{H}_2\text{O} \quad (4.60) \\
4 \text{S}_2 & \rightleftharpoons \text{S}_6 \quad (4.61) \\
3 \text{S}_2 & \rightleftharpoons \text{S}_6 \quad (4.62) \\
2 \text{S}_2 & \rightleftharpoons \text{S}_4 \quad (4.63)
\end{align*}
\]

Reaction (4.60) is called the reversed Claus reaction. The reaction rate of the reverse Claus reaction is suppressed as much as possible by the superclaus catalyst used (= sodium promoted 5 wt% Fe\textsubscript{2}O\textsubscript{3} catalyst on a silica support). This reaction would cause the reduction of \text{H}_2\text{S} conversion to sulfur. The reaction rate of superclaus is thus much larger than the reaction rate of the reverse Claus reaction.

The superclaus reaction (4.59) is a stoichiometric oxidation of hydrogen sulfide to sulfur. The hydrogen sulfide to oxygen concentration ratio should therefore be 2.

The operational temperature and pressure are 243.7 °C and 1.43 bar.
4.3.3.5 THE INCINERATOR

This is the last unit of the process scheme and in this unit all of the sulfur containing components are oxidized to sulfur dioxide. The following reactions occur:

\[
\begin{align*}
2 \text{S}_2 & \rightleftharpoons \text{S}_4 \quad (4.64) \\
3 \text{S}_4 & \rightleftharpoons 2 \text{S}_6 \quad (4.65) \\
4 \text{S}_6 & \rightleftharpoons 3 \text{S}_8 \quad (4.66) \\
\text{S}_4 + 8 \text{O}_2 & \rightleftharpoons 8 \text{SO}_2 \quad (4.67) \\
2 \text{H}_2\text{S} + 3 \text{O}_2 & \rightleftharpoons 2 \text{SO}_2 + 2 \text{H}_2\text{O} \quad (4.68) \\
2 \text{CO} + \text{O}_2 & \rightleftharpoons \text{CO}_2 \quad (4.69) \\
\text{CH}_4 + 2 \text{O}_2 & \rightleftharpoons \text{CO}_2 + 2 \text{H}_2\text{O} \quad (4.70) \\
2 \text{COS} + 3 \text{O}_2 & \rightleftharpoons 2 \text{CO}_2 + 2 \text{SO}_2 \quad (4.71) \\
\text{CS}_2 + 3 \text{O}_2 & \rightleftharpoons \text{CO}_2 + 2 \text{SO}_2 \quad (4.72) \\
2 \text{H}_2 + \text{O}_2 & \rightleftharpoons 2 \text{H}_2\text{O} \quad (4.73) \\
\text{S}_2 + 2 \text{O}_2 & \rightleftharpoons 2 \text{SO}_2 \quad (4.74)
\end{align*}
\]

In this step the temperature and pressure are respectively 706 °C and 1.22 bar.

4.3.3.6 KINETICS

The kinetics of the furnace of the superclaus section and the incinerator could not be found. However, it is assumed that the reaction rates are very fast because of the high temperatures in this unit. Also the furnace was modelled using thermodynamic equilibrium calculations. However some indications are observed that in the furnace of the superclaus section equilibrium is not totally obtained.

The kinetics of the catalytic Claus reactors could also not be found. Again these units were simulated using equilibrium calculations. In practice higher conversions of sulphur can be obtained by shifting the chemical equilibrium to the product side (e.g. selective removal of one of the products). Also the selectivity of the catalyst could not be taken into account. In the catalytic Claus reactors the Kaiser S-501 catalyst was used (see § 4.2.3.4).

The kinetics of the superclaus reactor could not be obtained from the literature. However the conversion of hydrogen sulfide and selectivities of the sodium promoted 5 wt% ironoxide catalyst on a silica support were known. These data were used to model the superclaus step. The superclaus reaction (reaction (4.59) in §4.3.3.4) was near to completion and simulated by using CHEMCAD. The remaining reactions were simulated by assuming chemical equilibria.

4.3.3.7 THERMODYNAMICS OF EQUILIBRIA

While operating most of the units (except for the reduction step of carbon dioxide and the absorption tower, in which the pressure is 25 bar) at low pressure, it was assumed, that the gases present, behaved as ideal gases. In these cases the ideal gas law can be used to predict the behaviour of the gases. To obtain the equilibrium constants K of the several reactions in a unit the following equations were used:
Conversions of the several different compounds can be calculated using mass balances and the formulas presented below.

\[ C_p = a + bT + cT^2 + d \frac{d}{T^2} \quad (4.75) \]

\[ S_T = S_{298.15} + \int_{298.15}^{T} \frac{C_p}{T} dT \quad (4.76) \]

\[ H_T = H_{298.15} + \int_{298.15}^{T} C_p dT \quad (4.77) \]

\[ \frac{G_T - H_{298.15}}{T} = -S_T - \frac{H_T - H_{298.15}}{T} \quad (4.78) \]

\[ \Delta H_{f,T} = \Delta H_{f,298.15} + (H_T - H_{298.15})_{\text{compound}} - \sum (H_T - H_{298.15})_{\text{elements}} \quad (4.79) \]

\[ \Delta S_{f,T} = S_{T_{(\text{compound})}} - \sum S_{T_{(\text{element})}} \quad (4.80) \]

\[ \Delta G_{f,T} = \Delta H_{f,T} - T\Delta S_{f,T} \quad (4.81) \]

\[ \ln K_T = -\frac{\Delta G_T}{R \cdot T} \quad (4.82) \]

Conversions of the several different compounds can be calculated using mass balances and the formulas presented below.

\[ \Pi (v_i) = P^{-v} \cdot K_T \quad (4.83) \]

\[ v = \sum v_i \quad (4.84) \]

\[ \sum a_{ij} v_j = b_i \]
Figure 4.6: Equilibrium between the molecular species of sulfur.
4.3.3.8 THE SEVERAL SULFUR SPECIES

It is known that in the gas phase several different sulfur modifications are present. The most important ones are: \( S_2 \), \( S_4 \), \( S_6 \) and \( S_8 \). Recent work [12] indicates that the sulfur species present in the vapour phase consist of \( S_3 \), \( S_5 \) and \( S_7 \) as well.

The temperature determines which sulfur modification occurs in the gas phase (this phenomenon can be seen in Figure 4.6. In the case of higher temperatures it can be seen that \( S_2 \) is present at the highest concentration. At lower temperatures (as is the case in the catalytic (super)Claus reactors and the sulfur condensors) sulfur will be present as \( S_8 \).

With the computer program CHEMSAGE it was possible to calculate which sulfur modification occurred to what extent. When sulfur is present in the liquid phase it consists of rings of \( S_8 \). This is the major reason why the assumption was made that only \( S_8 \) condensates as liquid phase while the \( S_6 \), \( S_4 \) and the \( S_2 \) present remain in the gas phase. The fraction of \( S_8 \) which remains in the gas phase can be calculated using the formulas presented below:

\[
x \cdot P_{S_8}^{cat} = y \cdot P
\]

\[
P_{S_8}^{cat} = \exp\left[\frac{-8.757 \cdot 10^3}{T} - 35.684 \cdot \frac{\ln(T)}{\ln(10)} + 11.058 \cdot 10^{-3} \cdot T + 109.05\right]
\]
Figure 5.1 Schematic drawing of the IFB system
5 PROCESS EQUIPMENT CALCULATIONS

In this chapter first the assumptions made and the chosen calculation methods are described. This is done for the main equipment. The other pieces of equipment like heatexchangers, pumps and compressors are described later in this chapter. The results can be found in the equipment specification sheets (Appendix 3) and the results of the modelling of the fluidized beds can be found in Appendix 10 and in Figure 5.1.

5.1 ASSUMPTIONS AND CALCULATION METHODS

Except for a description of the assumptions and calculation methods also a consideration of pressure and pressure drop is made.

5.1.1 IFB NOXSO UNIT

The main pieces of equipment in the IFB NOXSO Unit are the adsorber (R11 and R12), the heater (R18 and R19), the regenerator (R23 and R24) and the cooler (R28 and R29). These fluidized bed reactors are modelled according to Schouten [15] and are assumed to be adiabatic. The reactions in the adsorber and the regenerator are modelled by Ma [17]. For the heater and the cooler models are used, described by Kunii [20]. The equations of these models are described in §5.2.

The used sorbent particles properties can be found in Appendix 9.

The enthalpies of most streams are determined with the help of the computer program CHEMCAD. The thermodynamic model used is Soave Redlich Kwong. The enthalpy change of the sorbent in the cooler and the heater are determined with a listing of the Cp found in the databanks of the computer program ASPEN. The enthalpy of the sorbent in the streams to and from the IFB NOXSO Unit is neglected. This can be done because preliminary calculations point out that the solid loadings of these streams are very low. In fact, the particle loadings of these streams are that low, that those particles cannot be removed from the gas streams. According to table 10.11 of Coulson [21] the minimum particle loadings for solid-gas separations has to be at least 250 mg per m³ gas.

5.1.1.1 ATTRITION

The solids that are blown out of the beds are formed due to attrition. The assumed attrition rate is 0.01 kilogram per kilogram of solids in the bed and per hour of residence time.

According to Duisterwinkel [22] no attrition takes place in the dense beds of the system because $U_p = U_{mf}$ for the average particle size. The next equations were found in Duisterwinkel [22].
\[ \alpha \rightleftharpoons \frac{dm}{dt} = \frac{3k_a}{d^3}(U-U_m) \] 

(5.1)

\[ \alpha = 0.01 \text{ [wt\%/hr]} = 2.778 \times 10^{-8} \text{ [g/g*s]} \]

With the given equation the total attrition is calculated per bed:

\[ \Delta M = \alpha \tau M_0 \] 

(5.2)

Assumed is that the smallest particales formed due to attrition are 50 \mu m. There is also assumed that two third of the produced particles will leave the system in the cooler, where a special bed is placed to blow out all the particles that are smaller than 840 \mu m.

Another assumption is that the loss of NO\textsubscript{x}, SO\textsubscript{2} and SO\textsubscript{3} due to attrition can be neglected.

The computer program MathCAD has been used to make all the necessary calculations.

5.1.2 CONNECT AND SULFUR RECOVERY SECTION

All the reactions occurring in the several units of the sulfur recovery section (R32, R44, F64, R86, R72, F86 and the sulfur condensors) are assumed to be thermodynamic equilibria. This assumption was made because of lack of information obtained from literature about the kinetics of the several reaction steps. According to Biendarra [5] this assumption is near reality for the reduction of carbon dioxide to methane. The simulations of the reactions mentioned above are done by using the computer program CHEMSAGE. This program is capable of calculating thermodynamic equilibria.

The gases in the process streams are considered to be ideal gases. This can be done because of the low pressures the units are operated at.

The performance of the sulfur dioxide and the carbon dioxide reduction is optimized for maximum reduction by supplying sufficient hydrogen. The process conditions for the two reduction units, the Claus furnace, the incinerator and the two catalytic Claus converters are corresponding the data obtained from literature (§4.2). The operating temperature for the sulfur condensors is obtained from the NOXSO design.

Because of the fact that CHEMSAGE is limited to simulations containing only fifteen components, reactions occurring with ethane, propane and butane are neglected. These components only are present in low concentrations compared with the other components in the feed of the sulfur recovery section. The concentrations of ethane, propane and butane are thus considered to be constant.

During simulations the presence of ethane, propane and butane is taken into account by adding it to the nitrogen amount present in the process stream. Same is done for argon present in air (see below).
Assumptions made for the several sulfur species are mentioned in §4.3.3.8.

The absorber/stripper tower section has not been simulated at all. This is done because of lack of time. Here assumptions are made for the absorption (and stripping) performance of the tower section according to Kohl [6]. This way also the process conditions were obtained. The assumptions were made on the base of linear scale-up.

The furnace of the Claus section is considered to be isothermal.

The simulation of the superclaus unit is based on the work done by Terörde [3]. The superclaus catalyst is supposed to have an efficiency of 0.96 for the conversion of hydrogen sulfide to elemental sulfur. The overall conversion of hydrogen sulfide is 95%; so the conversion of hydrogen sulfide in the superclaus reaction would be: 0.96 * 0.95 = 0.91. The rest of the hydrogen sulfide is here assumed to be available for the other reactions in the superclaus step. For these reactions thermodynamic equilibria are assumed. These equilibria again were simulated using CHEMSAGE; the superclaus reaction was simulated using CHEMCAD (thermodynamics: SRK).

The air used in the designed plant is composed of the components mentioned in table 5.1. and is assumed to have a humidity of 70%.

Table 5.1. Composition of dry air used in the designed plant.

<table>
<thead>
<tr>
<th>Component</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>[-]</td>
<td>[vol%]</td>
</tr>
<tr>
<td>N₂</td>
<td>78.09</td>
</tr>
<tr>
<td>O₂</td>
<td>20.95</td>
</tr>
<tr>
<td>Ar</td>
<td>0.93</td>
</tr>
<tr>
<td>CO₂</td>
<td>0.03</td>
</tr>
</tbody>
</table>

5.1.3 PRESSURE CONSIDERATION

The pressures in the IFB NOXSO Unit are chosen and the pressure drops can be calculated. The pressure of the feed of the reduction step of sulfur dioxide is determined by the outlet pressure of the regenerator of the IFB process. The pressure drop over this tubular reactor was calculated with subjoined formula:
This way the pressure drops over the reduction step of CO₂ and the two catalytic Claus steps are determined as well. The pressure drop of the superclaus is assumed to be as big as the pressure drop of the catalytic Claus reactors.

The pressure drop of the heat exchangers is taken to be 0.028 bar according to the NOXSO design. For the pressure drop of the Claus furnace, the incinerator and the sulfur condensers, it is assumed that it has the same value.

The pressure of the feed of the Claus furnace has to be 1.9 bar to ensure that the pressure of the stack is big enough for easy stack discharge. The pressure of the stack therefore must be bigger than atmospheric pressure.

5.2 CALCULATIONS ON THE IFB NOXSO UNIT

This unit consists of interconnected fluidized beds. These are fluidized beds connected with each other by weirs and orifices. Now first the modelling of interconnected fluidized beds will be explained. Then the adsorber, heater, regenerator and cooler will be treated separately.

5.2.1 MODELLING OF INTERCONNECTED FLUIDIZED BEDS

For the modelling of fluidized beds the equations described by Schouten [15] are used.

The minimum fluidization velocity of fluidized beds can be calculated with the following Wen & Yu equation.

\[ U_{mf} \approx \frac{\eta_g}{d_p} \left( \sqrt{\frac{(33.7^2 + 0.0408 \times \rho_g \times d_p \times g)}{\rho_p \times (\rho_p - \rho_g) \times g}} \right) \]  (5.4)

In this equation the Archimedes number can be described as follows:

\[ A_r = \frac{\rho_p \times d_p^3 \times (\rho_p - \rho_g) \times g}{\eta_g^2} \]  (5.5)

Normally the values for the porosity of the bed at minimum fluidization conditions are between 0.40 and 0.50. Here \( \varepsilon_{mf} \) has been chosen 0.40.

The bubble size in a fluidized bed is also influenced by the porous distribution plate on the bottom of the bed. The next equation is used for the average bubble size.

\[ d_{avg} = 0.54 \times g^{-0.2} \times (U_0 - U_{mf})^{0.4} \times (0.4 \times H + 4 \times \sqrt{A_0})^{0.8} \]  (5.6)

In this equation \( U_0 \) is the superficial gas velocity. This velocity can be obtained by dividing the bottom surface of the bed \( A \) by the volume flow of the gas through the bed \( \phi_v \). Further the \( A_0 \) is the hole surface of the distribution plate and \( H \) is the height of the expanded fluidized bed. The plate will be blocked when the holes are about two times the diameter of the solids. A hole diameter as big as one particle causes a great
pressure drop. A hole diameter between these extremes was chosen. From Perry [13] the following equation was taken:

$$\phi_M = C_A \frac{2 \pi \rho g \Delta P}{\left(1 - \frac{A_f}{A_p}\right)^2}$$  \hspace{1cm} (5.7)

This equation can be used to calculate the pressure drop over the distribution plate.

The average velocity of the rising bubbles can be described by the equation of Davidson and Harrison.

$$U_{b Avg} = 0.711 \sqrt{g \rho_d d_{eff Avg}}$$  \hspace{1cm} (5.8)

Now the porosity of beds that are at more than minimal fluidization conditions can be calculated. This $\varepsilon_b$ can be calculated with the help of the following equation.

$$\varepsilon_b = \frac{U_0 - U_{mf}}{U_0 - U_{mf} + U_{b Avg}}$$  \hspace{1cm} (5.9)

The total porosity of beds that are at more than minimal fluidization conditions can be calculated as follows.

$$(1 - \varepsilon_{bed}) = (1 - \varepsilon_b)(1 - \varepsilon_{mf})$$  \hspace{1cm} (5.10)

This way the mass of solids in the beds $M_s$ can be calculated with the help of the porosity of the particle $\varepsilon$ which is 0.65.

$$M_s = H \pi A_0 (1 - \varepsilon)(1 - \varepsilon_b)(1 - \varepsilon_{mf}) \rho_s$$  \hspace{1cm} (5.11)

The last item that can be calculated for each fluidized bed is the pressure drop over this bed. The pressure drop $\Delta P$ can be calculated by using the next equation.

$$\Delta P = \rho_s \pi (1 - \varepsilon)(1 - \varepsilon_b)(1 - \varepsilon_{mf}) g H$$  \hspace{1cm} (5.12)

The next step is the orifice between a dense bed and the following lean bed. In order to retrieve a stream containing the sorbent stream $F_s$ a pressure drop is needed. This pressure drop $\Delta P_o$ can be calculated. The surface of the orifice $A_o$ can be determined. Now because of the pressure drop also a leak stream of gas will flow from the dense bed to the neighbouring lean bed as well. This stream can be calculated when the pressure drop and the surface of the orifice are known. These two
can be calculated with the following equations according to Snip [14].

\[ \Delta P_{o} \approx g \cdot H \cdot \rho_s \cdot [(1 - \varepsilon_{m}) - (1 - \varepsilon_s) + (1 - \varepsilon_m)] \quad (5.13) \]

\[ A_{o} = \frac{F_{s}}{C_{p} \cdot \sqrt{2 \cdot \rho_s \cdot [(1 - \varepsilon_m) \cdot \Delta P_{o}]}} \quad (5.14) \]

The part of the solids that flows through the IFB NOXSO Unit will be lost due to attrition. Because of attrition smaller particles will be formed and these can be blown out of the beds. In order to calculate the size of the particles that will be blown out the next method can be used. This method is described by Haider, Levenspiel and Kunii in [15].

According to this method first the dimensionless terminal velocity of a particle \( U_t \) must be calculated. Then with the help of a figure the dimensionless particle size \( d_p \) can be determined. This way the size of the particles that are blown out can be determined.

\[ U_t = U_t \left[ \frac{\rho_g^2}{\eta_s (\rho_s - \rho_g) \cdot g} \right]^{1/3} \quad (5.15) \]

\[ d_p = d_p \left[ \frac{\rho_g^2 (\rho_s - \rho_g) \cdot g}{\eta_s^2} \right]^{1/3} \quad (5.16) \]

In all the equations so far the temperature and pressure dependence can be put in by the viscosity \( \eta_{g} \) and the density \( \rho_{g} \) of the incoming gas streams. The used equations are the next two equations.

\[ \rho_g(T,P) = \frac{K \cdot P \cdot 10^5}{273.15 + T} \quad (5.17) \]

\[ \eta_g(P,T) = (K1 + K2 \cdot T + K3 \cdot P \cdot 10^5) \cdot 10^{-6} \quad (5.18) \]

The constants \( K, K1, K2 \) en \( K3 \) are obtained by fitting the viscosity data and the density data of every component by the last two equations. Then the constants are averaged according to the composition of the gas stream. The data are found in the data bank of CHEMCAD and Perry [13]. This way the pressure and temperature could
be altered during calculation with the aid of MATHCAD.

5.2.1.1 ADSORBER

In the lean bed of the adsorber the amount of sulfur dioxide to be adsorbed must be as large as possible to achieve an overall sulfur removal efficiency of at least 95%. The sulfur plant (= superclaus section) namely cannot remove all the sulfur that comes from the regenerator. For a 90% removal of NO\textsubscript{x} there is no complication. The gas leaving the adsorber is transported to the stack. The amount of sorbent needed to achieve this efficiency can be calculated as follows:

$$\left(\phi_{\text{mol, fluegas}} \cdot y_{\text{SO}_2, \text{in}} - \phi_{\text{mol, fluegas}} \cdot y_{\text{SO}_2, \text{out}}\right) \cdot M_s = \frac{F_s \cdot S_a}{100} - \frac{F_s \cdot S_f}{100}$$  \hspace{1cm} (s. 19)

With:

- $S_a = 1.5 \text{ wt\%}$
- $S_f = 0.3 \text{ wt\%}$
- $\phi_{\text{mol, fluegas}} = 7.13 \text{ kmole/s}$
- $y_{\text{SO}_2, \text{in}} = 2400 \cdot 10^{-6}$
- $y_{\text{SO}_2, \text{out}} = 72 \cdot 10^{-6}$
- $M_s = 32 \text{ kg/kmole}$

This gives a sorbent flow rate of 42.27 kg/s.

In the adsorber it is demanded that the gases NO\textsubscript{x} and SO\textsubscript{2} are removed by adsorption on the adsorber Al\textsubscript{2}O\textsubscript{3} with Na\textsubscript{2}O being the active sites. The amount of removal of the NO\textsubscript{x}SO\textsubscript{2} sorbent depends on temperature, sorbent properties, NO\textsubscript{x} and SO\textsubscript{2} concentrations, flue gas flow rate, reaction time, etc. An adsorption model is used which is based on the test results from the NO\textsubscript{x}SO\textsubscript{2} POC plant. A few assumptions were made:

1. The sorbent does not remove any NO\textsubscript{x} unless there is SO\textsubscript{2} in the flue gas.
2. The sorbed NO\textsubscript{x} will desorb from the sorbent if more SO\textsubscript{2} is fed into the reactor.
3. The spent sorbent, when heated to desorb all the NO\textsubscript{x} but not treated with regenerants to remove sulfur, loses its NO\textsubscript{x} removal ability.
4. The NO\textsubscript{x} and SO\textsubscript{2} sorption reaction is NO\textsubscript{x} sorption limited.

The model described in [17] is used to modelate the adsorber. The sorbent conversion factor is defined as follows:

$$X = X_0 + \frac{C_{\text{NO}_2 \cdot \text{Na}_2 \cdot \text{O}}} {C_t} + C_{\text{Na}_2 \cdot \text{SO}_3} + C_{\text{Na}_2 \cdot \text{SO}_2}$$  \hspace{1cm} (5.20)
This gives the fraction sites of the sorbent that are occupied by the pollutants. $X_0$ is the initial sorbent conversion factor, defined as:

$$X_0 = \frac{S_r}{3200 \cdot C_r} \quad (5.21)$$

This means that the sorbent is always occupied by this fraction of sulfur, $S_r$ in this equation is the sulfur content of the regenerated sorbent in wt%. 3200 is the sodium molecular weight times 100. From this an average sorbent conversion factor results from a time average scheme:

$$\bar{X} = 1 - \frac{F}{E} \cdot \left(1 - \frac{X_0 - \frac{F}{E}}{1 - \frac{F}{E}} \right) \quad (5.22)$$

$$D = 1 + K_1 \cdot P_x \cdot y_{SO_2} \quad (5.23)$$

$$E = (k_2 \cdot P_x \cdot y_{NO_x}^2 + k_3 + \frac{k_4}{K_1 \cdot K_2}) \cdot K_1 \cdot P_x \cdot y_{SO_2} \quad (5.24)$$

$$F = \frac{k_2}{K_2} \cdot P_x \cdot y_{SO_2} \cdot \left(1 - \frac{S_a}{3200 \cdot C_r} \right) \quad (5.25)$$

In which $S_a$ stands for the sulfur content of the sorbent leaving the adsorber in wt%, $y_{NO_x}$ is the mean gas fraction of NO, $y_{SO_2}$ is the mean fraction of SO$_2$ and $\tau$ is the sorbent residence time in seconds. This is only possible if $r_1 >> r_2, r_3$ and $K_1 >> 1$ and thereby the next equations can be used.

$$C_{Na_2OSO_4} = K_1 \cdot P_x \cdot y_{SO_2} \cdot C_{Na_2O} \quad (5.26)$$

$$C_{Na_2OSO_4} = k_3 \cdot C_{Na_2OSO_4} \cdot \tau \quad (5.27)$$
Using equation (5.22) with the above mentioned formulas and incorporated with the fluid-bed model of gas phase plug-flow and solid phase mixed-flow assumptions results in the adsorber model equation:

\[
\frac{F_g}{C_F F_s} \left[ \phi_a y_{Oa} + \frac{\phi_b}{2} y_{Ob} \right] = (1 - X_0 - \frac{F}{E}) \left( 1 - e^{\frac{-E}{D \frac{W_s}{F}}} \right)
\]  

(5.28)

In this equation also the residence time is present.

\[
\tau = \frac{W_{\text{solids}}}{F_s}
\]

(5.29)

At first the mean concentrations have to be defined as well as the total number of Na\textsubscript{2}O sites per kilogram sorbent:

\[
\bar{y}_{SO_2} = \frac{y_{SO_2} \Phi_{SO_2}}{\ln(1 - \Phi_{SO_2})}
\]

(5.30)

\[
\bar{y}_{NO_x} = \frac{-y_{NO_x} \Phi_{NO_x}}{\ln(1 - \Phi_{NO_x})}
\]

(5.31)

\[
C_t = \frac{1}{2} \times \frac{Na}{2300} + \frac{0.6 - 0.0075 \times T_a}{1000}
\]

(5.32)

When these are known the mass of solids in the beds can be calculated by rewriting equation (5.28):

\[
W_{\text{solids}} = -\frac{D \frac{F}{B}}{e} \ln(1 - \frac{F_g}{C_F F_s} \left( \phi_a y_{Oa} + \frac{\phi_b}{2} y_{Ob} \right))
\]

(5.33)

\[
F_s \left[ C_{ps} (T_1) T_1 - C_{ps} (T_{ar}) T_{st} \right] = F_g \left[ C_{ps} (T_p) T_{gr} - C_{ps} (T_1) \right]
\]

(5.34)
The dense bed of the adsorber does not have a function except for transporting the sorbent particles. Therefore this bed is modelled as a fluidized bed at minimum fluidization conditions. At this conditions the solids are transported the best way according to Korbee [16].

5.2.1.2 COOLER

The lean bed of the cooler will be used for actual cooling purposes. There are three different ways to model a cooler or heater: cross-flow, countercurrent flow and cocurrent. The last one is of no importance to this process because it is assumed that the other two flows have more influence on the cooling of the sorbent solids because the driving force ($\Delta T$) is bigger. The following energy balance is used for further calculations:

First one bed was calculated with cross-current flow and compared with two and three beds also in cross-current flow. It appeared that for three beds less air was needed and less space so the three beds system was taken and compared with three beds in cross-, counter-, cross-current flow.

The disadvantage of the counter-current flow is the large pressure drop. Another option is to get three beds with the first cross-, second counter- and the third cross-current. The result of comparing this with three cross-current beds following the method of [20] is that three cross-current beds are better.

The cooler also contains a bed where the smallest particles that are produced by attrition are removed. This is done by blowing an air stream at higher superficial gas velocity. The cooler was chosen for this purpose because the sorbent particles do not contain as much sulfur containing compounds as for example in the heater. In order to compensate for the loss of sorbent the dense bed will be used to add the fresh sorbent particles.

The dense bed of the cooler does not have a function in the IFB process, therefore it can be used to regulate the flow of solids in the system according to Korbee [16].

At first the bed was sized for $U_{mf}$. After this the effects on the dense bed were examined for a gas flow below $U_{mf}$.

The following happened:

When $e_{bed}$ decreases it causes the height of the bed to go down and the pressure drop to increase. This last effect causes the solids flow rate to increase, but less than it would increase based on the porosity of the bed only and not considering the bed height.

If $e_{bed}$ increases, the bed height increases also but the pressure drop decreases instead. The last effect causes the solids flow to decrease. Therefore the dense bed of the cooler is sized to regulate the solids flow and the velocity of the gas is below $U_{mf}$. 
For the dense bed:

Table 5.2. Data of the dense bed of the cooler

<table>
<thead>
<tr>
<th></th>
<th>R29 (with $U_{mf}$)</th>
<th>R29 (with new $U_0$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_{expand}$ [m]</td>
<td>1.73</td>
<td>1.73</td>
</tr>
<tr>
<td>$A$ [m$^2$]</td>
<td>11.63</td>
<td>11.63</td>
</tr>
<tr>
<td>$W$ [m]</td>
<td>11.63</td>
<td>11.63</td>
</tr>
<tr>
<td>$L$ [m]</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$P_{in}$ [kPa]</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>$T_{in}$ [$^\circ$C]</td>
<td>120</td>
<td>120</td>
</tr>
<tr>
<td>$T_{out}$ [$^\circ$C]</td>
<td>120</td>
<td>120</td>
</tr>
<tr>
<td>$\Delta P$ [kPa]</td>
<td>9.76</td>
<td>9.76</td>
</tr>
<tr>
<td>$U_0$ [m/s]</td>
<td>0.26</td>
<td>0.25</td>
</tr>
<tr>
<td>$U_{mf}$ [m/s]</td>
<td>0.26</td>
<td>0.26</td>
</tr>
<tr>
<td>$d_{pt}$ [$\mu$m]</td>
<td>127</td>
<td>125</td>
</tr>
<tr>
<td>$\varepsilon_{bed}$ [-]</td>
<td>0.40</td>
<td>0.40</td>
</tr>
<tr>
<td>$d_{b,max}$ [m]</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>$\tau_{gas}$ [s]</td>
<td>6.65</td>
<td>6.94</td>
</tr>
<tr>
<td>$\tau_{solid}$ [s]</td>
<td>96.10</td>
<td>96.10</td>
</tr>
<tr>
<td>$M$ [ton]</td>
<td>4.05</td>
<td>4.05</td>
</tr>
</tbody>
</table>
For the orifice:

**Table 5.3. Data of the orifice of the dense bed of the cooler**

<table>
<thead>
<tr>
<th></th>
<th>R29 (with ( U_{mf} ))</th>
<th>R29 (with new ( U_o ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_{orifice}{[m^2]} )</td>
<td>0.047</td>
<td>0.047</td>
</tr>
<tr>
<td>( \Phi_{orifice}{[kg/s]} )</td>
<td>0.167</td>
<td>0.161</td>
</tr>
<tr>
<td>( \Delta P_{orifice}{[kPa]} )</td>
<td>3.387</td>
<td>3.389</td>
</tr>
</tbody>
</table>

5.2.1.3 HEATER

Like the cooler, in the lean bed of the heater cross-current flow was chosen. Also the same energy balance was used. This time however the best configuration is to use only one bed. The reason for this is the extra requirement of an exit gas temperature of 680 °C. This for safety reasons.

The purpose of the dense bed of the heater is to strip the remaining sulfur compounds from the sorbent. This is done with steam with a pressure of 2 bar and 680 °C. Also this temperature was chosen for safety reasons.

This bed is modelled as fluidized bed at minimum fluidization.

5.2.1.4 REGENERATOR

In the lean bed of the regenerator the regeneration step takes place. For this step the model of the NOXSO regenerator is used. This model is described by Ma [17].

\[
\sqrt{S_F S_a} \frac{1}{2} \left[ 0.297 e^{\frac{2580}{T}} \right] t_r
\]

(5.35)

Here \( T \) is the absolute bottom-bed temperature of the sorbent particles in Kelvin. The \( t_r \) is the reaction time and is also the minimum average residence time of the sorbent particles. The bed load \( W \) can be calculated as:

\[
W = F_s t_r
\]

(5.36)

It is assumed that the model still can be used despite of the extreme dilution caused by the added nitrogen stream.

The dense bed is used as a stripping bed and is modelled as a fluidized bed at minimum fluidization conditions.
5.2.1.5 SIZING OF THE BEDS

The adsorber has been sized according to the dimensions of the NOXSO adsorber as described by Ma [17]. Because of the pressure drop over the orifice the height of the other beds have to be about the same height as the adsorber. When the efficiency of the IFB NOXSO Unit is increased the beds will become lower and therefore the pressure drop over the orifice will become smaller. The efficiency cannot become too big otherwise there will be difficulties keeping the sorbent fluidized. This way the only variable size of the lean beds that can be altered during calculation is the surface.

The sizing of the dense bedden can be done using the following two methods. The first is to use indications of the ratio of the needed surface of the dense bed over the surface of the orifice according to Korbee [16]. The second method is a graphical one. The lean beds of the adsorber, the heater, the regenerator and the cooler are drawn in one figure. In this figure the surfaces of the lean beds are adjusted in such a way that the whole unit forms almost a square. Then the dense beds can be drawn in and thus determining dense bed surfaces and sizes in a grafical manner. The obtained surfaces must be at least as big as the surfaces obtained by the first method.

5.3 CALCULATIONS ON THE CONNECT UNIT AND THE SUPERCLAUS SULFUR RECOVERY UNIT

5.3.1 THE REACTOR FOR THE REDUCTION OF SO\(_2\)

The dimensions of the reactor for the reduction of SO\(_2\) were estimated using the kinetics of [2]. In this article some data was presented which related the conversion of SO\(_2\) to the molar flow \(N_0\), the amount of catalyst present in the reactor \(w\). It was found for the obtained conversion that the catalyst to feed ratio \(w/N_0\) was 47.2 \((\text{hr} \cdot \text{g}_{\text{cat}})/\text{mol}\). The molar flow in the reactor was found to be 791.5 \(\text{mol/s} = 2.85 \times 10^6 \text{ mol/hr}\). This led to the following amount of catalyst present in the reactor \(w = 134 \times 10^6 \text{ g}_{\text{cat}}\). In the same article a typical bulk density was given \(\rho_b = 900 \text{ kg/m}^3\) which could be used to estimate the volume of the reactor \(V = 150 \text{ m}^3\). Because the length of the reactor affects the pressure according to (14) it was desirable that the length of the reactor was not to large. A diameter of 5 m and a length of 7.6 m were chosen.

5.3.2 THE REACTOR FOR THE REDUCTION OF CO\(_2\)

The reaction rate of reaction (4.19) was used to make an estimation of the volume of the reactor. This reaction rate was obtained from [5] and is presented below:

\[
r_{CO_2} = k_{CO_2} \cdot P_{CO_2}^{0.5} \cdot P_{\text{H}_2}^{0.4}
\]

(5.37)

The rate constant \(k_{CO_2}\) was found to be \(3.3 \times 10^{-3} \text{ m}^3/(s \cdot \text{kg}_{\text{N}_2} \cdot \text{bar}^{0.9})\).
The length of the reactor was determined by setting up a mass balance over the differential reactor. This led to the following equations:

\[ \phi_{mol}^{CA2} |_{x, dx} = \phi_{mol}^{CA3} |_{x} - r_{CA2} \cdot A \cdot dx \cdot M_{Ni} \]  

\[ \left[ \frac{2}{3} \cdot P_{CO2} \cdot \rho_{CO2} \cdot \rho_{pinc}^{CO2} \right] = -\left( \frac{\pi}{4} \cdot D^2 \right) \cdot K_{CO2} \cdot P_{H2}^{0.4} \cdot L^2 \cdot \left( \frac{\Phi_{v}}{R \cdot T} \right) \cdot \rho_{bed} \cdot wt\% \]  

It was assumed that the diameter of the reactor is \( D = 2 \) m. The following data were obtained from [5]:

\( \rho_{bed} = 1430 \text{ kg/m}^3 \) and \( wt\% = 40.0 \). Using the process conditions \( T = 632.88 \text{ K} \) and \( P_{tot} = 25.6 \text{ bar} \) the length of the reactor could be calculated. This resulted in \( L = 4.5 \text{ m} \) and thus in \( V = 14.2 \text{ m}^3 \).

5.3.3 THE ABSORPTION AND STRIPPER COLUMNS

Dimensions of the absorption and stripper columns were obtained from Kohl [6].

5.3.4 THE FURNACE OF THE CLAUS SECTION

Residence times for furnaces vary between 0.5 and 1.5 s, which depends on the \( H_2S \) concentration in the feed stream. A residence time of 1.0 s was chosen, with a flowrate of 3.0 \( m^3/s \) a volume \( V = 3.0 \text{ m}^3 \) was obtained.

5.3.5 THE CATALYTIC CLAUS REACTORS

The estimation of the volume of the catalytic claus reactors was made using a residence time of 4.0 s and a volumetric flowrate of the feed gas of 1.43 \( m^3/s \). The calculated volume was 5.7 \( m^3 \). This value had to be corrected by multiplying it by a factor 1.2, because of the presence of gas distribution plates and catalyst support layers. The corrected volume was \( V = 6.9 \text{ m}^3 \). With an estimation of the diameter \( D = 2 \text{ m} \) we calculated the length \( L = 2.2 \text{ m} \).

5.3.6 THE SUPERCLAUS REACTOR

The volume, length and diameter of the superclaus reactor were estimated by considering the same pressure drop over the superclaus reactor as over the Claus reactors. With this pressure drop and the bulk density of \( \rho_{bulk} = 900 \text{ kg/m}^3 \), it was possible to make an estimation of the length of the reactor, \( L = 2.0 \text{ m} \). If we assume that the diameter of this superclaus reactor is the same as the diameter of the Claus reactors, \( D = 2 \text{ m} \), the volume of the reactor can be calculated: \( V = 6.4 \text{ m}^3 \).
5.3.7 THE INCINERATOR

The incinerator was calculated analogously to the furnace of the Claus section. An estimation of the residence time inside the reactor was made: \( \tau = 1.0 \text{ s} \), with a volumetric flowrate of 4.4 m\(^3\)/s, the volume of the incinerator was found to be 4.4 m\(^3\).

5.4 CALCULATION OF DIMENSIONS AND PARAMETERS FOR HEATEXCHANGERS

An attempt was made to make an energy integration analysis as presented by Douglas [23] (the energy integration analysis according to Hohmann). The minimum heating and cooling requirements were calculated and the pinch temperature was determined. The temperature-enthalpy diagrams and the grand composite curve (Appendix 7) were constructed. The next step is the design of minimum-energy heatexchanger networks. Because the amount of streams considered in this energy analysis was so large, it was decided to couple streams with each other on geometrical reasons (and of course the first and the second law), this solution could be realized easier within the time available.

<table>
<thead>
<tr>
<th>Table 5.4. Basic data obtained from the energy integration analysis.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Minimum hot utility [MW]</td>
</tr>
<tr>
<td>Minimum cold utility [MW]</td>
</tr>
<tr>
<td>Pinch temperature [K]</td>
</tr>
</tbody>
</table>

Five types of heatexchangers were considered:
1) The normal heatexchanger in which one of the process streams transfers heat to the other.
2) The cooler, in which a process stream has to be cooled with water or another fluid.
3) Condensers, in which a total or a part of a process stream is condensed, the cooling medium used is usually water.
4) Flashers, in which the process stream (or a part of it) is vaporized.
5) Waste heat boilers, in which steam is generated from water by transfer of heat from a process stream.

Two different versions of heatexchangers were used:
1) The U-tube and
2) the binary pipe or double pipe heatexchanger.
Other versions could not be used because they were not suitable for high pressures (a chance of leakage), they were difficult to clean or they were not suitable for high temperature differences. Which versions to be used depends on the correction factor \( F_t \). The U-tube has the advantage that it is smaller than the binary pipe, but because an economic heatexchanger design cannot normally be achieved if the correction factor \( F_t \)
falls below 0.75, the binary pipe had to be chosen when the correction factor $F_t$ for the U-tube was less than 0.75.

The choice, whether a certain stream was led through the pipe or the shellside, depended on:
1) The most corrosive stream was led through the pipeside.
2) The stream with the highest pressure was also led through the pipeside.
3) The fluid that has the greatest tendency to foul the heat transfer surfaces should be placed in the pipeside.
4) If the fluid temperatures are high enough to require the use of special alloys, placing the higher temperature fluid in the tubes (pipeside) will reduce the overall cost.
5) The massflow of the two streams (largest massflow through the pipeside).

Another important aspect involved the number of heat exchangers needed. This was calculated using values for standard diameters and lengths. It was determined how many heat exchangers must be placed in parallel if these values were exceeded.

5.4.1 WASTE HEAT BOILER

An example for the calculation of the dimensions and characteristic parameters of a waste heat boiler is given below. In this example waste heat boiler H62 is considered. The process stream, which must be cooled, is led through the shellside, while the generated steam is led through the pipeside.

The excess heat of the process stream was used to heat cooling water to its boiling point, to evaporate it and then to superheat this saturated steam. In this waste heat boiler high pressure steam is generated (40 bar). The cooling water is subjected to the following changes:
1) Heating of the cooling water from 20°C to its boiling temperature of 250°C.
2) Evaporation of water to steam at 250°C.
3) Superheating of this saturated steam to 410°C.

The accompanying energy effects will be calculated below:

$$\Delta H = C_p \ast \Delta T$$

With $C_{p\text{water}} = 4.18*10^3 \text{ J/(kg*}^\circ\text{C)}$ it is calculated that $\Delta H_1 = 968.1 \text{ kJ/kg}$. The heat of vaporization was found in the steam tables: $\Delta H_2 = 1712.9 \text{ kJ/kg}$. The third heat effect is calculated using $C_{p\text{HP Steam}} = 3.0*10^3 \text{ J/(kg*}^\circ\text{C)}$. Resulting in $\Delta H_3 = 478.5 \text{ kJ/kg}$. The total enthalpy change will be $\Delta H_{tot} = \Delta H_1 + \Delta H_2 + \Delta H_3 = 3159.5 \text{ kJ/kg}_{\text{water}}$. The energy transfer from the process stream to the generated steam was 134.68 kW, so it is possible to determine the amount of cooling water necessary, which is of course equal to the amount of steam generated.

$$\phi_{m\text{water}} = \frac{\Delta H_{process\text{-stream}}}{\Delta H_{tot}}$$

(5.41)
It is calculated, that the amount of cooling water necessary is \( \dot{m}_{\text{water}} = 0.0426 \text{ kg/s}. \)

Two temperature trajectories occur in the waste heat boiler:

1. Saturated steam is superheated from 250°C to 410°C at 40 bar in the first trajectory, while the process stream was cooled from 55°C to \( T_{\text{intermediate}} \).

2. The process stream was cooled from \( T_{\text{intermediate}} \) to 221.85°C in the second trajectory, while the cooling water was heated from 20°C to 250°C. Also water evaporated to steam in this trajectory at 250°C.

The following heat balances can be made from which it is possible to calculate the relevant parameters in every trajectory:

\[
Q_1 = \dot{m}_{\text{water}} \Delta H_3 =
\]

\[
= C_p \dot{m}_{\text{process stream}} \left( T_{\text{entrance}} - T_{\text{intermediate}} \right)
\]

(5.42)

\[
Q_2 = \dot{m}_{\text{water}} (\Delta H_1 + \Delta H_2)
\]

(5.43)

Calculated was \( Q_1 = 20.4 \text{ kW}, Q_2 = 114.3 \text{ kW} \) and \( T_{\text{intermediate}} = 506.2°C \). Other relevant parameters are the logarithmic temperature difference (LMTD) \( \Delta T_{\text{LM}} \), the correction factor \( F_t \), the corrected LMTD \( \Delta T_m \) and the heat exchanging surface area \( A \).

For the binary pipe or double pipe heat exchanger was found that \( F_t = 1 \). The formula for the calculation of the correction factor was only valid for the U-tube. Subjoined formulas were used to determine these parameters:

\[
\Delta T_{\text{LM}} = \frac{(T_1 - T_2) - (T_2 - T_1)}{\ln \frac{(T_1 - T_2)}{(T_2 - T_1)}}
\]

(5.44)

\[
F_t = \sqrt{R^2 + 1} \ln \left( \frac{1 - S}{1 - R \cdot S} \right)
\]

(5.45)

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

(5.46)

\[
S = \frac{(T_2 - T_1)}{(T_1 - T_2)}
\]

(5.47)
\[ \Delta T_m = Ft \times \Delta T_{im} \]  
(5.48)

\[ Q = U \times A \times \Delta T_m \]  
(5.49)

These equations were applied and delivered the following results:

1 Traject 1: \( F_t = 1 \) (binary pipe), \( \Delta T_{im} = \Delta T_m = 196.4^\circ C \) and \( A_1 = 3.46 \text{ m}^2 \) with \( U = 30 \text{ W/(m}^2\text{\circ C)} \).

2 Traject 2: \( F_t = 1 \), \( \Delta T_{im} = \Delta T_m = 227.8^\circ C \) and \( A_2 = 3.14 \text{ m}^2 \) with \( U = 160 \text{ W/(m}^2\text{\circ C)} \).

The overall heat exchanging coefficient \( U \) was 30 W/(m\(^2\)\circ C) in the first traject because gas/gas heat exchange is involved here, while in the second traject liquid/gas heat exchange is involved with \( U = 160 \text{ W/(m}^2\text{\circ C)} \).

The total heat exchanging surface area was \( A_{ot} = A_1 + A_2 = 6.60 \text{ m}^2 \), while the LMTD over the whole heat exchanger (not only the two trajects) had a value of \( \Delta T_{im} = \Delta T_m = 173.1^\circ C \).

It has to be mentioned, that waste heat boiler H10 was incorrectly modelled. This waste heat boiler is the link between the IFB-process and the Claus section. The enthalpies in the IFB-process were determined with Chemcad and those of the Claus-section were determined with Chemsage. This introduced an error, because both programs use different thermodynamical constants and thus both programs will calculate different enthalpies for the same streams.

5.4.2 THE CONDENSORS

Calculation of the characteristic parameters of the condensers was done in the same way as the waste heat boilers were modelled. In fact it was again two trajects, but the main difference was that the temperature at the exit of the tube was equal to the condensation temperature of the substance involved. This means that the traject, in which was dealt with liquid/liquid heat transfer (condensate/water), was so small, that it was neglected. Another point was that only a small part of the process stream is condensed, so the main heat transfer had to deal with gas/liquid heat exchange. The overall heat exchanging coefficient was \( U = 850 \text{ W/(m}^2\text{\circ C)} \). Horizontal condensers with condensation in the shellside and the cooling medium in the pipeside were used (most common configuration).

5.4.3 THE EVAPORATORS

Again the equations (5.44) to (5.49) were used, the heating medium was steam and the overall heat exchanging coefficient \( U \) was estimated (160 W/m\(^2\)\circ C).

5.4.4 THE COOLERS

The coolers were modelled using an overall heat exchanging coefficient of \( U = 160 \text{ W/(m}^2\text{\circ C)} \) for liquid/gas heat transfer, cooling medium was almost always water.
5.4.5 THE HEAT EXCHANGERS FOR THE PROCESS STREAMS

In this case, when a process stream transfers heat to another one, almost always gas/gas heat transfer was involved, with the accompanying overall heat exchanging coefficient $U = 30 \text{ W/(m}^2\text{oC)}$. Data for heat exchanger H53 could not be found in the literature.

5.4.6 CALCULATION OF THE ENERGY REQUIREMENTS OF THE FIRED HEATERS

Direct fired exchangers were used, when very high temperatures were required. These fired heaters were heated with natural gas. The amount of natural gas needed was calculated using the heat of combustion of natural gas: $\Delta H_r = 54.626 \text{ MJ/kg}$. In case of fired heater F7 0.24 MW had to be supplied. Resulting in a natural gas feed of 0.0044 kg/s.

5.5 CALCULATION OF THE DIMENSIONS OF THE LIQUID-VAPOUR SEPARATORS

The liquid-vapour separators concerned in this process were all so called knock-out drums. These knock-out drums were modelled using the method of Coulson [21]. For small flowrates vertical liquid-vapour separators can be used. Liquid-vapour separating efficiencies near 100% can be obtained. An example of the calculation of the dimensions of knock-out drums is given below for liquid-vapor separator V66. The first parameter to be calculated is the maximal design vapor velocity $\dot{u}_v$, which can be calculated using formula (5.51):

$$U_{v,max} = 0.035 \sqrt{\frac{\rho_f}{\rho_v}}$$

In the first L/V separator $\rho_f = 1788 \text{ kg/m}^3$ and $\rho_v = 1.40 \text{ kg/m}^3$ and thus $\dot{u}_v = 1.25 \text{ m/s}$. If the vapour volumetric flowrate is known, then the minimum vessel area and vessel diameter can be determined using equations (5.51 and 5.52).

$$A_{min} = \frac{\phi_v}{U_{v,max}}$$

$$D_{min} = \sqrt{\frac{4*A_{min}}{\pi}}$$
\( \Phi = 0.94 \, \text{m}^3/\text{s} \), and thus \( A_{\text{min}} = 0.75 \, \text{m}^2 \) and \( D_{\text{min}} = 0.98 \, \text{m} \). The disengagement space is equal to this diameter. With the known liquid volumetric flowrate and the volume for 10 min hold up, the liquid depth can be calculated. The liquid volumetric flowrate equalled \( 194 \times 10^{-6} \, \text{m}^3/\text{s} \), so the volume for 10 min hold up \( V \) was 0.12 \, \text{m}^3. The liquid depth can be calculated by dividing the volume for 10 min hold up by the minimum area.

\[
H_i = \frac{V_i}{A_{\text{min}}} \quad (5.53)
\]

This resulted in a liquid depth of \( H_i = 0.16 \, \text{m} \). The chosen dimensions were
- Height \( H = 1.1 \, \text{m} \)
- Diameter \( D_{\text{min}} = 0.98 \, \text{m} \)
- Volume \( V = 0.75 \, \text{m}^3 \)

The liquid/gas separators V26 and V31 however are computed with the help of the program CHEMCAD.

5.6 CALCULATIONS ON PUMPS AND COMPRESSORS

Pumps and compressors are computed with the help of the program CHEMCAD. The efficiencies used are obtained from Douglas [23]
6 MASS AND ENERGY BALANCE

The mass balance and the energy balance can be found in Appendix 2. The compositions of the streams can be found in Appendix 6.
7 SPECIFICATIONS OF THE USED EQUIPMENT

In Appendix 3 the specification sheets of all the used equipment can be found.
8 PROCESS CONTROL

All compressors and expanders in this process have a pressure controller so the discharge pressure is determined.

8.1 PROCESS CONTROL OF IFB PROCESS

The coal burner (power plant furnace) needs sufficient air. The air supply is regulated by putting a flow control over the heater recycle to the power plant and the power plant air feed. The power plant air feed will be determined by measuring the composition of the recycle of the heater.

The solids flow in the system is controlled by the transport bed of the cooler. This bed is limited by taking the operating gas flowrate lower than the minimum fluidisation. Changing conditions in the flue gas will cause a change in the gas flowrate of the air into the cooler and thereby the flowrate of the dense bed of the cooler.

In this case it is better to let the dense bed of the heater be the controlling bed because of the recycle loop over the cooler. The reflux air flowrate depends namely on the incoming air flowrate. The dense bed of the heater does not have any influence on the modelling of the heater and also this bed can be taken to regulate the solids flow.

Every bed has a pressure controller. The control takes place by measuring the pressure in the free board zone of the beds.

In the adsorber a water spray is installed to control the temperature in the bed.

The air feed of the heater needs to be preheated. This air feed temperature will be controlled by a temperature controller over the furnace.

To control the composition of the outgoing process stream of the regenerator two feed ratio controllers are installed. The first one is placed on the recycle loop from the absorption tower in the sulfur recovery section and the incoming natural gas stream. The second one is placed on the incoming natural gas stream and the incoming steam stream. Also the nitrogen supply is determined by a flow controller.

The air feed stream of the cooler is controlled by the flow controller which is connected to the flow controller of the flue gas stream and to the gas stream entering the dense bed of the cooler. By controlling the solids rate the absorption can be controlled.

The incoming temperature of the air recycle from the cooler to the beds will be controlled by a temperature controller.

8.2 THE PROCESS CONTROL OF THE SULFUR RECOVERY SECTION

A feed ratio controller is installed over the $SO_2$-reduction step to control the composition of the outcoming process stream. The same is done for the $CO_2$-reduction step.

After the absorption tower a pressure controller is installed in the rich solution stream to regulate the pressure.

The stripping efficiency of the stripper tower is controlled by installing a flow controller over the rich solution stream and the incoming steam stream. This means that the outcoming process stream will be of a constant composition. The lean solution stream is recycled to the absorption tower. Regulation of the incoming pressure is accomplished by a pressure control in the lean solution stream. A level controller
controls the water reflux at the top of the stripper tower. In the reboiler at the bottom of the stripper tower the temperature is controlled by a temperature controller.

The air feed of the furnace of the Claus section needs to be preheated. This air feed temperature will be controlled by a temperature controller over the furnace.

To make sure the incoming process stream of the Claus furnace is at constant temperature a temperature control is installed over the furnace in the process stream. A feed ratio controller is used to control the composition of the outgoing process stream.

To make sure the incoming process stream of the Claus furnace is at constant temperature a temperature control is installed over the furnace in the process stream. A feed ratio controller is used to control the composition of the outgoing process stream.

The temperature in the sulfur condensation steps after the Claus furnace, the two catalytic Claus reactors and the superclaus reactor is controlled by temperature controllers over the process streams going into the gas-liquid separators and the cooling water. This way the efficiency of the following conversion step to sulfur will kept constant by controlling the sulfur condensation.

Depending on the concentration of oxygen in the process stream flowing into the incinerator the air supply to the super Claus reactor is regulated by the quality control and also by the maximum flow regulated by the flow controller. The same quality controller is connected to a flow controller positioned on the air supply for the incinerator to make sure that the emission standards are not exceeded.
9 PROCESS SAFETY

9.1 SAFETY

On the IFB system a permanent control on the fluidization conditions is necessary because if the gas flow will fall back the fluidized bed will become a packed bed this leads to hot spots especially in the adsorber (exothermic reactions).

The natural gas stream in the regenerator is also a factor of concern. A fall back of the gas stream here will cause a gas leak to the heater. In contact with oxygen it will cause fire. Therefore the dense bed of the heater is stripped with water and the temperature is above the flame temperature of natural gas. The natural gas will burn immediately.

Nitrogen needs a special cryogenic vessel because it is easier to store it as a liquid.

The properties (like toxicity, explosion limits) of the substances, which are important for the process, are reported in Appendix I. Most of these substances are toxic.

Most reaction steps in the sulfur recovery section operate under atmospheric pressure. Only the carbon dioxide reduction step and the absorption tower in the recycle loop between the IFB section and the sulfur recovery section operate at moderate pressure (25 bar).

Furthermore two units in the sulfur recovery section work at high temperatures. The Claus furnace work at 1028 °C and the incinerator work at 706 °C.

In both cases (pressure and temperature issue) working personnel should be instructed well.

The reduction step of carbon dioxide and the reduction step of sulfur dioxide use hydrogen; therefore caution should be taken to prevent explosions and/or fire by air-contact.

Also caution should be taken while renewing the catalyst in the reduction steps of carbon dioxide and sulfur dioxide. Then also the hydrogen must be protected against air/oxygen.

To prevent the emission of sulfur substances other than sulfur dioxiden excess air has to be supplied to the incinerator. This air supply has to be regulated well and is done by a cascade control of a quality controller and a flow controller over the outcoming stream of the superclaus unit and the air stream entering the incinerator.

Storage of hydrogen should be done under certain preconditions. First of all hydrogen is kept at 12 bar and -242 °C in a cryogenic tank. Secondly, fire should be avoided nearby the hydrogen storage tank (and the two reduction steps of sulfur dioxide and carbon dioxide.

Hydrogen is very explosive and flammable when it is in contact with nitrogen oxides and air/oxygen.

The storage of sulfur should be done in a closed tank which consists of sulfur-resistant steel. The incoming sulfur in the storage tank must be sprayed by ammonia to prevent the formation of polysulfides, which produces a nasty smell. This formation is caused by the presence of small concentrations of hydrogen sulfide in the sulfur product stream of the plant.
9.2 HEALTH

While in the designed plant hydrogen, nitrogen oxides, sulfur dioxide and hydrogen sulfide is used, personnel working near the reactors should be protected. MAC values should also not be exceeded.
MAC values and other properties of substances in the plant are reported below:

9.3 ENVIRONMENTAL ASPECTS

Because of environmental regulations national standards for the emission of sulfur dioxide and carbon dioxide preconditions are present for the emission of the plant.

However it must be noticed that unexpected emissions somewhere in the plant can cause that the national emission standards are exceeded. The possibilities of these unexpected emissions for example, by breakage of pipes, should be minimized by frequently checking of the equipment.

National standards for emission are mentioned in the conclusions.
Figure 10.1 Process scheme of the Taylor calculation of the IFB system

Figure 10.2 Process scheme of the Taylor calculation of the S-recovery system
10 ECONOMIC ANALYSIS

The survey of the economic analysis is mentioned in appendix 5.

10.1 INVESTMENT COSTS ACCORDING TO TAYLOR

In this method the total process/plant is divided into several process steps. To every process step/ process stream points are given. With the total amount of points \( S_i \) given to the process, the costliness-index is determined. The costliness-index depends on the extremes in throughput, material, temperature and pressure.

The costliness-index \( f \) is calculated by:

\[
f = \sum_{i=1}^{N} (1,3)^{S_i}
\]  \hspace{1cm} (10.1)

With the costliness-index the investments depending on the production are calculated:

\[
I_B = 45 \cdot f \cdot P^{0.39} \cdot \frac{C_t}{300}
\]  \hspace{1cm} (10.2)

\( I_B \) = Investments in process units [k€]
\( P \) = Production
\( C_t \) = Year index [24]

In the developed process two main products are produced. In the section of the plant containing the IFB part 'clean' air is produced; in the sulfur recovery section of course the product is sulfur. Therefore the plant is divided into two separate parts. For each part a Taylor investment analysis was made. The figures 10.1 and 10.2 contain the schemes of the two parts.

From table 10.1 and 10.2 it is found that \( f_{IFB} = 19.2 \) and \( f_{S_{rec.}} = 6.7 \). The production capacity ('clean' air production capacity) of the IFB part is \( 6.20 \cdot 10^3 \) kton/y; the production capacity (sulfur production capacity) of the sulfur recovery part is \( 1.46 \cdot 10^1 \) kton/y.
Table 10.1. Process modelling according to Taylor (IFB part)

<table>
<thead>
<tr>
<th>Streams</th>
<th>throughput</th>
<th>material</th>
<th>P/T</th>
<th>total</th>
<th>f</th>
</tr>
</thead>
<tbody>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>1.0</td>
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<td>1.0</td>
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<td>0</td>
<td>-2</td>
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</tr>
<tr>
<td>U2</td>
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<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>U3</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Process steps</th>
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<th>P/T</th>
<th>total</th>
<th>f</th>
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<td>1.5</td>
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<td>0.9</td>
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<td>D</td>
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<td>-</td>
<td>-</td>
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Table 10.2. Process modelling according to Taylor
(sulfur recovery part)

<table>
<thead>
<tr>
<th>Streams</th>
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<th>material</th>
<th>P/T</th>
<th>Total</th>
<th>f</th>
</tr>
</thead>
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<td>1</td>
<td>1</td>
<td>4</td>
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<table>
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<th>Process steps</th>
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<th>material</th>
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<th>f</th>
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</thead>
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<td>5</td>
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<td>F</td>
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<td>0</td>
<td>2</td>
</tr>
<tr>
<td>D</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>4</td>
</tr>
</tbody>
</table>
Therefore using equation (10.2) the total investment costs:
\[ I_{B,\text{tot}} = I_{B,\text{FB}} + I_{B,\text{rec.}} = 37,905 \text{ k£ (UK 1995)} = 94,002 \text{ k£ (NL 1995)} \]

**10.2 INVESTMENT COSTS ACCORDING TO LANG/HOLLAND**

The total investment costs are determined by using Lang's factor method. The Lang factors used are calculated by Holland's method.

The investment costs of the equipment (without supports) are multiplied by the Lang factor in order to compensate for pipes, installation, engineering etc:

\[ C_i = f_L \cdot C_e \]  \hspace{1cm} (10.3)

\[
\begin{align*}
C_i &= \text{Investment costs (fixed capital)} \\
 f_L &= \text{Lang factor} \\
 C_e &= \text{Equipment costs without supports}
\end{align*}
\]

The value of the Lang factor is determined by using data from the process industry [24]. The costs of the equipment without supports is determined by using figures [21] or calculated by empiric equations. This method takes the material used, power and dimensions of the equipment into account.

The used correlations and figures determine the costs in 1979; corrections for these costs are done by using a cost index of 162. This cost index is based on published values of the cost indices in the 'Webci prijzenboekje' [25] and corrected by assuming 6% inflation in the last two years in Holland.

**10.2.1 COMPRESSORS/PUMPS**

The costs of the compressors and the pump used are calculated by the following correlation [21]:

\[ C_e = 700 \cdot P^{0.8} \]  \hspace{1cm} (10.4)

\[
\begin{align*}
 C_e &= \text{Investment costs without supports [£]} \\
 P &= \text{Power [kW]}
\end{align*}
\]
10.2.2 EXPANDERS

The calculation of the investment costs for the expanders are determined by using the six-tenth rule [23]:

\[ I = I_0 \cdot \left( \frac{C}{C_0} \right)^m \]  \hspace{1cm} (10.5)

- \( I \) = Investment costs
- \( I_0 \) = Investment costs known equipment
- \( C \) = Capacity
- \( C_0 \) = Capacity of known equipment
- \( m = 0.6 \).

The known equipment has a capacity of 0.9 MW and costs 473 k£.

10.2.3 FURNACES, TANKS, GAS/LIQUID SEPARATORS, HEATEXCHANGERS AND VESSELS

The costs of the furnaces, tanks, gas/liquid separators, heatexchangers and vessels are determined by using different figures [21]. The determined costs are on the base of material and pressure requirements.

10.2.4 TOWERS

The total cost of the towers consists of the costs of a vertical vessel plus the total costs of the plates and the raschig rings (pack) [21].

The cost of the plates depends on the type of plate, the plate diameter and material used.

10.2.5 REACTORS, SEAL PITS AND STACK

The costs of the reactors, seal pits and the stack are determined using the 'Weboi prijzenboekje' [25]. The costs are determined on base of the dimensions of the equipment.

The costs of the IFB reactors (R11 - R29, table 10.3) contain also the costs of the sorbent present after the plant build-up, just before the start-up. This cost also can be considered to be part of the working capital. Here it is considered to be part of the fixed capital.
The calculated costs per equipment and the used Lang factors are presented in table 10.3.

**Table 10.3. Equipment costs without supports and Lang factors used.**

<table>
<thead>
<tr>
<th>Equipment code</th>
<th>Costs</th>
<th>Lang factor</th>
</tr>
</thead>
<tbody>
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<td>[-]</td>
<td></td>
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<td>Compressor C3</td>
<td>6855</td>
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<td>C27</td>
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<td>H47</td>
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<td>H50</td>
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<tr>
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<tr>
<td>H51</td>
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<td>-</td>
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<td>H56</td>
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<td>H62</td>
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<td>F64 (waste heat boiler)</td>
<td>70</td>
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</tr>
<tr>
<td>H65</td>
<td>6</td>
<td>3.5</td>
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<tr>
<td>H69</td>
<td>6</td>
<td>3.5</td>
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<tr>
<td>H73</td>
<td>6</td>
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<tr>
<td>H78</td>
<td>6</td>
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<td>H83</td>
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<td>H85</td>
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<tr>
<td>R12</td>
<td>30</td>
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<tr>
<td>R18</td>
<td>609</td>
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<tr>
<td>R19</td>
<td>35</td>
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<td>Equipment code</td>
<td>Costs</td>
<td>Lang factor</td>
</tr>
<tr>
<td>----------------</td>
<td>--------</td>
<td>-------------</td>
</tr>
<tr>
<td>[kf]</td>
<td>[ ]</td>
<td></td>
</tr>
<tr>
<td>R28</td>
<td>307</td>
<td>2.7</td>
</tr>
<tr>
<td>R29</td>
<td>30</td>
<td>2.7</td>
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<tr>
<td>R32</td>
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<tr>
<td>R44</td>
<td>131</td>
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<tr>
<td>R68</td>
<td>90</td>
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<td>R72</td>
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<td>2.7</td>
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<tr>
<td>R77</td>
<td>90</td>
<td>2.7</td>
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<tr>
<td>Seal pit M67</td>
<td>68</td>
<td>3.2</td>
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<tr>
<td>M71</td>
<td>68</td>
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<tr>
<td>M75</td>
<td>68</td>
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<td>M80</td>
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<td>3.2</td>
</tr>
<tr>
<td>Stack M87</td>
<td>77</td>
<td>3.0</td>
</tr>
<tr>
<td><strong>TOTAL COSTS:</strong></td>
<td></td>
<td><strong>255093 kf</strong></td>
</tr>
<tr>
<td>(Lang included)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
10.3 TOTAL INVESTMENT COSTS ($I_T$)

The total investment costs ('once off') of a plant consists of the fixed capital ($I_F$), the miscellaneous capital ($I_L$) and working capital ($I_W$). The fixed capital normally is 80% of the total investment costs; the miscellaneous capital 14% of the total investment costs; the working capital 6% of the total investment costs.

The fixed capital consists of the costs for the equipment plus installation, piping, control (instruments), buildings, engineering, cost estimation, construction etc. The miscellaneous capital consists of the costs for licencies, know-how, pre-operational expenses and start-up (working capital items excluded). The working capital is build up out of the costs for start-up until income starts.

The fixed capital is determined above by two different methods; Taylor method: $I_F = 94,002,000$; Lang/Holland method: $I_F = 255,093,000$. The Lang/Holland method is much more detailed than the Taylor method. Therefore the fixed capital calculated by the Lang/Holland method is used for further calculations.

So: $-I_F = 255,093,000$
$-I_L = 44,641,000$
$-I_W = 19,132,000$

$-I_T = 318,866,000$

10.4 TOTAL COSTS OF A PRODUCT PER COST PLACE ($K_T$)

The total production costs ($K_T$) for a processing plant consists of the processing costs ($K_F$) and the general costs ($K_A$). The processing costs is the sum of the direct production costs ($K_D$) and the indirect production costs ($K_I$).

The direct production costs is the sum of the variable costs ($K_V$), the semi-variable costs ($K_S$) and the fixed costs ($K_F$). The variable costs is composed of the costs made for raw material, steam, energy, cooling and auxilaries. The semi-variable costs is the sum of the labour costs and the costs for equipment repair. The fixed costs ($K_F$) is the sum of the write off for the total investment costs ($I_T$), cost for interest and the insurance costs.

The general costs ($K_A$) is composed of costs for marketing, administration, research and development.

The indirect costs consists of costs made for items involving the plant site not mentioned above.
10.4.1 PROCESSING COSTS ($K_p$)

10.4.1.1 DIRECT PRODUCTION COSTS ($K_0$)

10.4.1.1.1 VARIABLE COSTS ($K_p$)

The costs for the raw materials and auxiliaries are mentioned in table 10.4.

**Table 10.4 Variable costs**

<table>
<thead>
<tr>
<th>Item</th>
<th>Price</th>
<th>Consumption</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>[-]</td>
<td></td>
<td></td>
<td>[kʃ/y]</td>
</tr>
<tr>
<td>Sorbent</td>
<td>6.11f/kg</td>
<td>4.3e-3kg/s</td>
<td>757</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>0.3f/m³</td>
<td>0.36kg/s</td>
<td>13</td>
</tr>
<tr>
<td>Natural gas</td>
<td>0.24f/Nm³</td>
<td>0.67Nm³/s</td>
<td>4634</td>
</tr>
<tr>
<td>Process water</td>
<td>1.0f/ton</td>
<td>1.84kg/s</td>
<td>53</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>5.0f/kg</td>
<td>0.12kg/s</td>
<td>16560</td>
</tr>
<tr>
<td>Cooling water</td>
<td>0.15f/m³</td>
<td>5.8e-2m³/s</td>
<td>248</td>
</tr>
<tr>
<td>High pressure steam</td>
<td>35f/ton</td>
<td>0.25kg/s</td>
<td>249</td>
</tr>
<tr>
<td>Low pressure steam</td>
<td>28f/ton</td>
<td>3.5kg/s</td>
<td>2800</td>
</tr>
<tr>
<td>Electricity</td>
<td>0.08f/kWh</td>
<td>7.98e7kWh</td>
<td>6381</td>
</tr>
<tr>
<td>Catalyst (Sulfur recovery section)</td>
<td>2250f/m³</td>
<td>185m³/4y</td>
<td>104</td>
</tr>
</tbody>
</table>

* The assumption was made that the catalyst for the $SO_2$ reduction step, the $CO_2$ reduction step, the two catalytic Claus converters and the superclaus unit has to be renewed every four years.

The prices were obtained from the 'Webci prijzenboekje' [25], from the PEP Yearbook [26] and from data given by the NOXSO cooperation.

The total variable costs is f31,800,000.
10.4.1.1.2 SEMI-VARIABLE COSTS ($K_j$)

The equipment repair costs are considered to be 3% of the fixed costs ($I_F$): $f7,653,000$.

The labour costs are calculated using the Wessel equation:

$$\frac{h}{P} = k \cdot \frac{N}{C^{0.76}}$$  \hspace{1cm} (10.6)

$k = 0.97 \text{ [-]} (1995)$

$h =$ Number of working hours $[\text{h}]

N = Number of production steps $[-]

C = Production capacity per day $[\text{ton/day}]$

The $k$-value is a constant and based on a value in 1986; this value is corrected considering a raise in production of 6% per year [24].

With the Wessel equation the man hours per ton of product is determined. This value has to be multiplied by the number of tons of product produced per hour. Finally the latest determined value has to be multiplied by the number of hours the plant is in process per year ($8000 \text{ h/y}$) and by the personnel costs per man hour to obtain the total labour costs per year. The personnel costs per man hour is set to $f55$. Using this value the costs for holidays, social costs etc. are considered as well. The labour costs are $f1,105,000$.

The total semi-variable costs are $f8,758,000$.

10.4.1.1.3 FIXED COSTS ($K_f$)

The fixed cost consists of the interest to be paid for the total investment costs ($I_T$), the write off for the equipment and the insurance costs. The ratio of the interest and the costs for write off to the distribution of these costs over the amount of years the plant is written off depends on the chosen method for write off.

Here the rectilinear write off method [24] is used and the write off time is 10 years. Using the rectilinear write off method every year a fixed amount of money is written off. Therefore the value of the plant will decline linearly in time. This amount is determined using the following equation:

$$R_x = \frac{a-s}{n}$$  \hspace{1cm} (10.7)

$R_x =$ Annual write off

$a =$ Value of the plant at the begin of the write off

$s =$ Value of the plant at the end of the write off
The value of the plant at the beginning of the plant is the total investment costs "once off" ($I_p$). The value of the plant at the end of the write off time is equal to the multiplication of the value of the plant at the beginning times the annuity factor. This way also the relative devaluation of money in time is considered.

The annuity is calculated by:

\[
An = \frac{j}{1 - \frac{i}{(1 + i)^n}}
\]

(10.8)

- $An$ = Annuity factor
- $i$ = Interest
- $n$ = Write off time

Using an interest of 8% the annuity factor is 0.149. The annual write off cost therefore is $f27,136,000$. The cost for interest is 8% of the total investment costs ($I_p$): $f25,509,000$.

The insurance cost is about 1% of the fixed capital ($I_r$): $f2,551,000$.

The fixed costs are thus $f55,196,000$.

10.4.1.2 INDIRECT PRODUCTION COSTS ($K_o$)

The indirect production costs composed of 4% of the total investment costs ($I_r$) and 45% of the labour costs [24].

The direct costs are $f13,252,000$

10.4.2 GENERAL COSTS ($K_e$)

The general costs can be estimated by taking 5% of the earnings [24]. The general costs are $f69,000$.

10.5 EARNINGS

The earnings consist of the selling of the sulfur produced. The annual earnings are $f1384,000$ for a annual sulfur production of $1.46e4$ ton/y and a sulfur cost price of $51$/ton [26].

Considering the costs of the product per cost place ($K_r$) and a total sulfur production capacity of $1.46e4$ ton/y the virtual cost price of the produced sulfur would be $f7,476/ton$. The actual sulfur price is $f94.9/ton$. 
10.6 ECONOMICAL CRITERIA

The calculation of the economical criteria is done to compare alternative projects based on investments and costs.

10.6.1 RETURN ON INVESTMENT (ROI)

The ROI method is a simple engineering method in which the net profit will be divided by the total investments. Lower taxes are not considered in the preliminary stage of the factory.

\[
ROI = \frac{W}{I_F + I_W} \times 100\% \quad (10.9)
\]

- \( W \) = Profit
- \( I_F \) = Fixed capital
- \( I_W \) = Working capital

In this case the profit is negative and therefore taxes are not considered here. The ROI is negative and equals -39.27% for a market price of $94.86 per ton of sulfur.

10.6.2 INTERNAL RATE OF RETURN (IRR)

With the IRR method the return percentage is calculated in which the sum of the negotiated cash flows during the project stage equals zero. A project stage of ten years is chosen and one year to build the factory (year 0) is invested. The taxes are taken zero because the profit is negative. After the dismantle of the factory, the working capital and the not written off value of the factory are released. The calculation method can be found in Appendix 4. With a market price of $94.86 per ton of sulfur, the IRR is -34.48%.
11. CONCLUSIONS, DISCUSSION AND SUGGESTIONS

The main purpose, to remove 90% of the nitrogen oxides and 95% of the sulfur dioxide, is not reached for the sulfur dioxide. The efficiency of the sulfur dioxide removal is only 93.11%. The reason is that in the sulfur recovery unit equilibria are used to model the reactions. This way the selectivity of the catalysts are not considered. In practice the efficiency of the sulfur recovery unit could be over 99%.

During modelling the sulfur dioxide removal efficiency of the IFB NOXSO Unit is chosen 97%. This is done because of the expected lower efficiency of the sulfur recovery section. Repeated calculations with different adsorption efficiencies would result in a better overall sulfur recovery efficiency. This however could not be accomplished in this short period of time.

Emissions of sulfur dioxide, nitrogen oxides and particles to the atmosphere and the emission standards in Holland are presented in table 11.1. It can be seen that the emission standard for sulfur dioxide is exceeded because of the insufficient sulfur yield of the designed plant. Emission standards for carbon dioxide have not been found.

Table 11.1. Emission standards and emissions

<table>
<thead>
<tr>
<th>Component</th>
<th>Emission standards</th>
<th>Emission</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[mg/MJ]</td>
<td>[mg/MJ]</td>
</tr>
<tr>
<td>SO₂</td>
<td>250</td>
<td>500</td>
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<tr>
<td>NOₓ</td>
<td>180</td>
<td>73.3</td>
</tr>
<tr>
<td>particles</td>
<td>18</td>
<td>2.0</td>
</tr>
</tbody>
</table>

The economical side of this PDA does not have any satisfactory results either. The Rate On Investment is -39.27% and the Internal Rate of Return -34.48%. The process therefore cannot be economically justified. There are some reasons for this result. The first reason is that the solely product is originally a waste product. It will always be a non-profitable process. The second reason is the high costs of process equipment. Especially the hydrogen used in both the reduction steps and the absorption/stripping towers. Besides the reduction step of carbon dioxide to methane and the absorption tower of the tower section operate at 25 bar and deal with large process streams, therefore the costs relating to the increase of pressure are huge.

There are some things that need some attention. First the NOₓ recycle to the coal combustor of the power plant. In this PDA is assumed that the recycle does not have any influence on the composition of the flue gas. This is not true. In practice the NOₓ fraction in the flue gas will increase. In order to remove 90% of that NOₓ stream the IFB NOXSO Unit would become larger and thus more expensive and more difficult to keep the bed fluidized.

The second point is the fact that the sorbent particles cannot be removed from the gas streams because of the low fractions of the solids in the gas streams. If solids are present in the NOₓ recycle stream the particles will be burnt in the coal combustor.
Also the particles that leave the adsorber and leave the plant via the stack will cause no trouble. The solids that leave the cooler will cause a little holp up in the air recycle around the cooler. There are two possibilities for these particles to leave the unit. One possibility is via the dense bed of the adsorber and the other is together with the water that leaves the unit in the L/V separator (V31). Most harmful however are the particles that are blown out of the regenerator and will plug the packed catalyst bed of the reductors.

Another point is that the flue gas in practice will contain particles. Normally electrostatic precipitators are used to remove these particles. In real the solid stream that leaves the adsorber will be larger and thus a electrostatic precipitator will be needed right after the adsorber.

Another fact to be considered is that the furnace of the Claus section is assumed to be isothermal. This is not correct, it should be modelled as an adiabatic reactor.

Also problems are found within the connect section. Enthalpies calculated with CHEMCAD and CHEMSAGE are coupled in this section, both programs delivered different values for the enthalpy, this is the reason why heat exchanger H10 is modelled incorrectly. In order to prevent these errors modelling should be done in one program in future.

A way to make the designed process economically efficient is to create a system in which companies pay the cleaning plant to clean their waste gases. In future this kind of system could be created because of raising costs of gas cleaning in order to meet the environmental standards. If the cleaning company is able to clean the gases cheaper this might be successful.
### 12. EXPLANATION OF USED SYMBOLS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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</thead>
<tbody>
<tr>
<td>$\alpha$</td>
<td>rate constant of attrition</td>
<td>[kg/(kg*s)]</td>
</tr>
<tr>
<td>$\Delta G_{i,T}$</td>
<td>Gibbs free energy of formation at temperature $T$</td>
<td>[kJ/mol]</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>enthalpy change</td>
<td>[J/mol]</td>
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<tr>
<td>$\Delta H_{i,T}$</td>
<td>heat of formation at temperature $T$</td>
<td>[kJ/mol]</td>
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<td>$\Delta H_{i,298}$</td>
<td>heat of formation at 298.15</td>
<td>[kJ/mol]</td>
</tr>
<tr>
<td>$\Delta H_{r,298.15}$</td>
<td>standard heat of reaction</td>
<td>[kJ/mol]</td>
</tr>
<tr>
<td>$\Delta P$</td>
<td>pressure drop</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$\Delta P_o$</td>
<td>pressure drop over a orifice</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$\Delta S_{i,T}$</td>
<td>entropy of formation at temperature $T$</td>
<td>[kJ/(mol*K)]</td>
</tr>
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<td>$\Delta T$</td>
<td>temperature difference</td>
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</tr>
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<td>[$^\circ$C]</td>
</tr>
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<td>$\Delta T_m$</td>
<td>corrected LMTD</td>
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</tr>
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<td>viscosity</td>
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</tr>
<tr>
<td>$\eta_g$</td>
<td>gas viscosity</td>
<td>[Pa.s]</td>
</tr>
<tr>
<td>$\nu$</td>
<td>overall stoichiometric coefficient</td>
<td>[-]</td>
</tr>
<tr>
<td>$\nu_i$</td>
<td>stoichiometric coefficient</td>
<td>[-]</td>
</tr>
<tr>
<td>$\rho_b$</td>
<td>bulk density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_{bulk}$</td>
<td>density of the bulk stream</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_{cat}$</td>
<td>density of the catalyst</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_g$</td>
<td>gas density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_l$</td>
<td>liquid density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_p$</td>
<td>particle density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_s$</td>
<td>sorbent density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\rho_v$</td>
<td>vapour density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\tau_{gas}$</td>
<td>gas residence time</td>
<td>[s]</td>
</tr>
<tr>
<td>$\phi_m$</td>
<td>mass flow</td>
<td>[kg/s]</td>
</tr>
<tr>
<td>$\phi_{mol}$</td>
<td>molar flow</td>
<td>[mol/s]</td>
</tr>
<tr>
<td>$\phi_{mol,i}$</td>
<td>molar flow of component $i$</td>
<td>[mol/s]</td>
</tr>
<tr>
<td>$\phi_v$</td>
<td>volumetric flowrate</td>
<td>[m$^3$/s]</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>thermodynamic constant</td>
<td>[J/(mol*K)]</td>
</tr>
<tr>
<td>$A$</td>
<td>area</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$A_{heating}$</td>
<td>heat exchanging area</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$A_0$</td>
<td>surface of a hole of the distribution plate</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$A_T$</td>
<td>total free area of holes of a distribution plate</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$A_{IT}$</td>
<td>auto ignition temperature</td>
<td>[$^\circ$C]</td>
</tr>
<tr>
<td>$A_{min}$</td>
<td>minimum area</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$A_o$</td>
<td>surface of a orifice</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$A_p$</td>
<td>total cross-sectional area of the perforated distribution plate</td>
<td>[m$^2$]</td>
</tr>
<tr>
<td>$Ar$</td>
<td>Archimedes number</td>
<td>[-]</td>
</tr>
<tr>
<td>$b$</td>
<td>thermodynamic constant</td>
<td>[J/mol]</td>
</tr>
<tr>
<td>$c$</td>
<td>thermodynamic constant</td>
<td>[(J*K)/mol]</td>
</tr>
<tr>
<td>$C$</td>
<td>orifice coefficient</td>
<td>[-]</td>
</tr>
<tr>
<td>$C_{i}$</td>
<td>concentration of component $i$</td>
<td>[wt%]</td>
</tr>
<tr>
<td>$C_p$</td>
<td>specific heat</td>
<td>[J/(mol*K)]</td>
</tr>
<tr>
<td>$C_{p,g}$</td>
<td>specific heat of gas</td>
<td>[kJ/(mol*K)]</td>
</tr>
<tr>
<td>$C_{p,s}$</td>
<td>specific heat of solid</td>
<td>[kJ/(mol*K)]</td>
</tr>
</tbody>
</table>
d thermodynamic constant \[\text{[J/(mol\cdot K^3)]}\]
D diameter \[\text{[m]}\]
\(d = d_p\) particle diameter \[\text{[m]}\]
\(d_{\text{max}}\) maximum bubble size \[\text{[m]}\]
\(d_{\text{eqAvg}}\) equivalent average bubble diameter \[\text{[m]}\]
\(dm = \Delta M\) average mass loss in time \(\tau_s\) \[\text{[kg]}\]
\(D_{\min}\) minimum diameter \[\text{[m]}\]
\(d_p\) dimensionless particle diameter \[\text{[-]}\]
\(d_{pt}\) size of particle that is blown out at terminal velocity \[\text{[m]}\]
\(dt = \tau_{\text{solids}} = \tau\) residence time of the sorbent \[\text{[s]}\]
\(F_S\) sorbent mass flow \[\text{[kg/s]}\]
\(F_t\) correction factor \[\text{[-]}\]
g gravitational constant \[\text{[m/s^2]}\]
\(g_c\) dimensional constant \[\text{[m/s^2]}\]
\(G_T\) Gibbs free energy \[\text{[kJ/mol]}\]
H height of a fluidized bed \[\text{[m]}\]
\(H_0\) standard enthalpy \[\text{[kJ/mol]}\]
\(H_{298.15}\) enthalpy at 298.15 K \[\text{[kJ/mol]}\]
\(H_{\text{expand}}\) expanded bed height \[\text{[m]}\]
\(H_l\) liquid depth \[\text{[m]}\]
\(H_T\) enthalpy at temperature \(T\) \[\text{[kJ/mol]}\]
K \(K_1\) equilibrium constant \[\text{[1/atm]}\]
K \(K_2\) reaction constant \[\text{[1/(s\cdot \text{atm})]}\]
K \(K_2\) equilibrium constant \[\text{[1/atm]}\]
K \(K_3\) reaction constant \[\text{[1/s]}\]
K \(k_{\text{CO2}}\) reaction rate constant of \(\text{CO}_2\) \[\text{[m}^3/(s\cdot \text{kg}_{\text{Ni}}\cdot \text{bar}^0.8]}\]
k \(k_s\) rate constant \[\text{[-]}\]
K \(K_T\) equilibrium constant at temperature \(T\) \[\text{[-]}\]
L length \[\text{[m]}\]
LEL-UEL lower explosion limit- upper explosion limit \[\text{[vol\%]}\]
M molar mass \[\text{[g/mol]}\]
m \(m_0\) total mass of the fluidized bed \[\text{[kg]}\]
MAC maximum allowable concentration \[\text{[ppm]}\]
M \(M_{\text{Ni}}\) mass of Ni \[\text{[kg]}\]
M \(M_{\text{solids}} = W_{\text{solids}}\) mass of solids in the fluidized bed \[\text{[kg]}\]
N \(N_0\) molar flow \[\text{[mol/s]}\]
P total pressure \[\text{[Pa]}\]
P \(P_{\text{CO2}}\) partial pressure of \(\text{CO}_2\) \[\text{[bar]}\]
P \(P_{\text{H2}}\) partial pressure of \(\text{H}_2\) \[\text{[bar]}\]
P \(P_{\text{in}}\) inlet pressure \[\text{[Pa]}\]
P \(P_{\text{sals}}\) saturated vapour pressure of \(S_8\) \[\text{[Pa]}\]
P \(P_{\text{tot}}\) total pressure \[\text{[bar]}\]
Q heat transfered \[\text{[W]}\]
R dimensionless temperature ratio \[\text{[-]}\]
R \(R_{\text{gasconstant}}\) gas constant \[\text{[J/(mol\cdot K)]}\]
\(r_{\text{CO2}}\) reaction rate of \(\text{CO}_2\) \[\text{[-]}\]
\(\rho_{\text{air}}\) density of substance relative to air \[\text{[-]}\]
\(\rho_{\text{water}}\) density of substance relative to water \[\text{[-]}\]
S dimensionless temperature ratio \[\text{[-]}\]
\( S_0 \) standard entropy \[ \text{[J/(mol*K)]} \]
\( S_{298.15} \) entropy at 298.15 K \[ \text{[kJ/(mol*K)]} \]
\( S_a \) sulfur load after the adsorber \[ \text{[wt%]} \]
\( S_r \) sulfur load after the regenerator \[ \text{[wt%]} \]
\( S_T \) entropy at temperature \( T \) \[ \text{[kJ/(mol*K)]} \]
\( t \) time \[ \text{[s]} \]
\( T \) temperature \[ \text{[K]} \]
\( t_1 \) entrance temperature of the cold stream \[ \text{[K]} \]
\( T_1 \) entrance temperature of the hot stream \[ \text{[K]} \]
\( t_2 \) exit temperature of the cold stream \[ \text{[K]} \]
\( T_2 \) exit temperature of the hot stream \[ \text{[K]} \]
\( T_b \) boiling temperature \[ \text{[°C]} \]
\( T_{g,i} \) inlet gas temperature \[ \text{[K]} \]
\( T_{in} \) inlet temperature \[ \text{[K]} \]
\( T_m \) melting temperature \[ \text{[°C]} \]
\( T_{out} \) outlet temperature \[ \text{[K]} \]
\( U \) overall heat exchanging coefficient \[ \text{[W/(m²*K)]} \]
\( U_s \) superficial gas velocity in a fluidized bed \[ \text{[m/s]} \]
\( U_{Avg} \) superficial gas velocity at \( H = 0 \) \[ \text{[m/s]} \]
\( U_{mf} \) superficial gas velocity at minimum fluidization conditions \[ \text{[m/s]} \]
\( U_t \) terminal velocity \[ \text{[m/s]} \]
\( U_\ast \) dimensionless superficial velocity \[ \text{[-]} \]
\( \bar{u}_v \) maximal design vapour velocity \[ \text{[m/s]} \]
\( V \) volume \[ \text{[m³]} \]
\( V_i \) liquid volume for 10 min hold up \[ \text{[m³]} \]
\( w \) amount of catalyst \[ \text{[g_{cat}]} \]
\( w/N_0 \) catalyst to feed ratio \[ \text{[hr*g_{cat}/mol]} \]
\( W \) mass solid in fluidized bed \[ \text{[kg]} \]
\( wt\% \) weight percentage of Ni in the cat. \[ \text{[-]} \]
\( X \) sorbent conversion factor \[ \text{[-]} \]
\( X_0 \) initial sorbent conversion factor \[ \text{[-]} \]
\( x_i \) molar liquid fraction of component \( i \) \[ \text{[-]} \]
\( y_i \) molar vapour fraction of component \( i \) \[ \text{[-]} \]
\( \varepsilon \) particle porosity \[ \text{[-]} \]
\( \varepsilon_b \) bubble porosity \[ \text{[-]} \]
\( \varepsilon_{mf} \) porosity of fluidized bed at minimum fluidization conditions \[ \text{[-]} \]
\( \varepsilon_{tot} \) total porosity of a fluidized bed \[ \text{[-]} \]
13 REFERENCES


20. Kunii & Levenspiel, "Fluidization Engineering", p 421


of freedom.

If necessary, select additional design decision variables and plot the economic potential for the recycle structure flowsheet versus a relevant design decision variable.

The economic potential for the recycle structure takes into account the annualised, installed cost of the reactor as the only major equipment item. This latter cost ($C_R$) is given as:

$$C_R = 2.0 \times 10^3 \times (\text{Reactor volume})^{0.558} \quad [\text{in }$/$(m^3 \text{ yr})]$$

4. Structure of separation section.

Sketch your best guess of a separation system.

Guess whether a vapour recovery system might be needed, where it should be placed and what type might be best.

Guess the distillation sequencing alternatives that might be best.

Delft, 9 March 1994

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PROCESS SCHEME OF THE IFB PROCESS AND THE S-RECOVERY

AME SCHRAM AJ STOL
FVD nr: 3153
M KETING RM HOOGVLIET JAN. 1996

Streamnr. Temp. (°C) Abs. pressure (kPa)