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Conceptual Process Design

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Delft University of Technology

Subject

Design of a modified GO-Finer

Final report

Proprietary Information

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Abbreviations

RX1	Current Reactor 1 (guard reactor)
RX2	Current Reactor 2
RX3	New Reactor 3
HPHS	High Pressure Hot Separator
LPHS	Low Pressure Hot Separator
HPCS	High Pressure Cold Separator
SW	Sour Water
MEA	Methyl Ethanol Amine
DCMR	Dienst Centraal Milieubeheer Rijnmond
SS	Stainless Steel
CS	Carbon Steel
MO	Micro Organism
HDS	Hydro Desulphurization
DBT	DiBenzoThiophene
DMDBT	DiMethylDiBenzoThiophenes
DDS	Direct Desulphurization
HYD	Hydrogenation
NiMo	Nickel Molybdenum
PFS	Process Flow Scheme
API	American Petroleum Institute
HAZOP	Hazard and Operability Study
NFPA	National Fire Protection Agency
F&E Index	Fire and Explosion Index
(R01)	Reactor Vessel 1 (guard reactor, current RX1)
(R02)	Reactor Vessel 2 (modified current RX2)
(R03)	Reactor Vessel 3 (new reactor)
(P01)	Pump 1 (new pump)
(E01)	Heat Exchanger 1 (new heat exchanger)
(E02)	Heat Exchanger 2 (new heat exchanger)
(E03)	Heat Exchanger 3
(E07)	Heat Exchanger 7
(E08)	Heat Exchanger 8
(E09)	Heat Exchanger 9
(E10)	Heat Exchanger 10
(D01)	Drum 1 (current HPHS)
(D02)	Drum 2 (current LPHS)
(D03)	Drum 3 (current fractionator)
(D04)	Drum 4 (current fractionator overhead flash-vessel)
(D05)	Drum 5 (current Distillate side-stripper)
(D06)	Drum 6 (current flash vessel)
(D07)	Drum 7 (current HPCS)
(D08)	Drum 8 (current MEA scrubber)
(C01)	Compressor 1 (current compressor)

Summary

The main objective of this feasibility study is to investigate methods to decrease the sulphur content of the Distillate product stream of the GO-finer unit at the Rotterdam plant site of ExxonMobil. It is expected that future legislation will demand lower sulphur content in oil refinery products.

In this report several methods are described briefly. After a technical and economical evaluation one process option is chosen. In this option, an additional fixed bed reactor is installed. This reactor will operate in semi counter-current operation with the current hydrocracking and desulphurization reactor. To facilitate this, the current reactor needs to undergo some adjustments.

New equipment, i.e. two heat-exchangers and a reactor, needs to be installed.
For designing this new reactor an extensive simulation using Matlab ® has been done, to attempt to model the reactions occurring. The simulation of the GO-finer with exception of the reactor system is done with Aspen ®. Because the composition of the GO-finer feed is not completely determined, pseudo components are used.

The simulations and the economic evaluation of the results revealed that the total investment costs are rewarding (M$3.-), however the annual operating costs (M$105.- per year) are by far the determining economic factor. This is caused by the hydrogen consumption. It is recommended to further investigate possibilities to reduce the hydrogen consumption. Validation of provided information would be the first step. The changes of the current process suggested and explained in this report will not make additional profit. However, if future legislation demands low sulphur content additional costs are inevitable.
Also additional research can be done to reduce the hydrogen consumption, which will also reduce the costs.

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1 Introduction

In 1958 Esso Nederland B.V. started the construction of the Refinery Rotterdam, which was officially opened in May 1960. Mayor adjustments to the original refinery were the installation of the Flexicoker (mid 80's) and the installation of a Hydrocracker (mid 90's).

1.1 Unit description.

The GO-finer unit is part of this refinery. It was originally designed to desulphurize the coker gas oil stream. A block scheme that represents the part of the refinery were the GO-finer unit is located is given in Figure 1.1.

The vacuum Distillate bottoms are sent to a Flexicoker, where it is converted into fuel gas, LPG, naphtha and coker gas oil (LKGO and HKGO). These KGO streams have a high metal, sulphur and poly-aromatic content and need to be treated by a hydrotreating unit: the GO-finer. The main product streams are the GO-finer Distillate, with a maximum S-content of 2500 ppm, and the GO-Finate, with a maximum of 10 000 ppm S. The Distillate is blended into heating oil and the GO-Finate serves as hydrocracker feedstock.

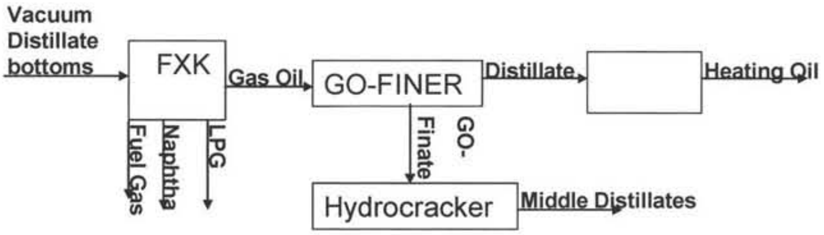


Figure 1.1: Block scheme of the current refinery operation

The current GO-finer unit consists of multiple stages. These stages are given in the block scheme of Figure 1.2. The feed is mixed with hydrogen and sent to the reaction section. From the reaction section the process stream goes to the separation section where the vapour process stream is routed to the H_2 work-up section. Hydrocarbons still present in the vapour process stream are recycled to the separation section.

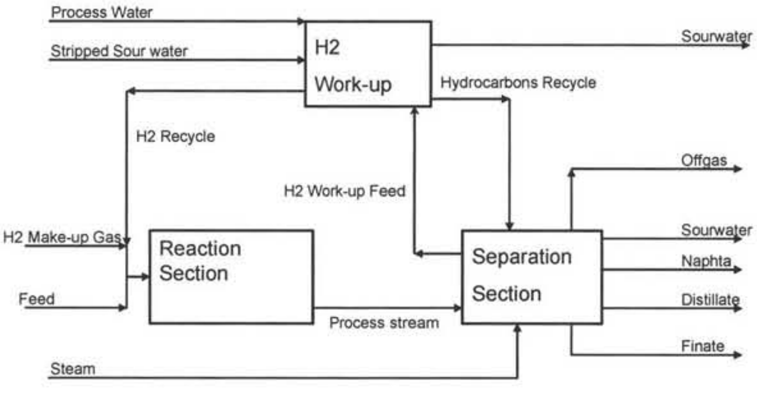


Figure 1.2: Block scheme of the different process stages in the GO-finer unit

The reaction section consists of two separate reactors, RX1 and RX2. In RX1 the metals are removed. In RX2, a fixed bed reactor with four catalyst beds, hydrodesulphurization and some mild hydrocracking takes place. The reactor effluent is sent to the separation section. In a high pressure and hot separator (HPHS), most of the formed H_2S is removed. After the HPHS the liquid hydrocarbon stream is sent to a low pressure hot separator (LPHS), which separates heavy and light fractions, to optimize the subsequent fractionation. The H_2 work-up feed is sent to the H_2 work-up where it is treated by a high pressure cold separator (HPCS). The hydrogen gas is separated for recycle. A stream containing hydrocarbons is returned to the fractionator and sour water is sent to the SW-stripper. The hydrogen gas is sent to a MEA scrubber, which removes any residual impurities (mainly H_2S). A block scheme of this process is represented in Figure 1.3.

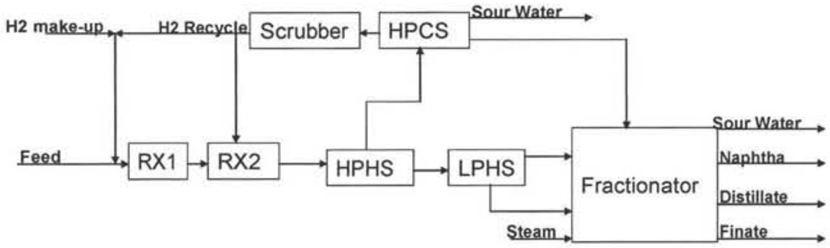


Figure 1.3 Block scheme of current GO-finer operations

1.2 Product information

As the Distillate stream is blended into heating oil, which will generate the most profit, this final product will be the subject of some analysis.

Heating oil is very similar to diesel fuel, and both are classified as Distillates. It consists of a mixture of petroleum-derived hydrocarbons in the 14- to 20-carbon atoms range. That is, heating oil's chemical formula is usually either $C_{14}H_{30}$, $C_{15}H_{32}$, $C_{16}H_{34}$, $C_{17}H_{36}$, $C_{18}H_{38}$, $C_{19}H_{40}$, or $C_{20}H_{42}$. Heating oil is used as a fuel for diesel motors and heating installations. In the Netherlands however, heating oil is no longer used that much for heating. The heating oil that is used as fuel for diesel engines is coloured to ensure the heating oil isn't used as conventional fuel for cars.

Heating oil can be produced in several grades:

-Heavy heating oil; this oil is very viscous. It is used mainly for heating of ships

-Semi-heavy heating oil; this oil is slightly lighter. It is used mainly for heating in industry.

-light heating oil; an even lighter heating oil. It is used as heating oil in houses and ships.

-Diesel oil; the lightest heating oil. It is used as fuel for ships, trucks and tractors.

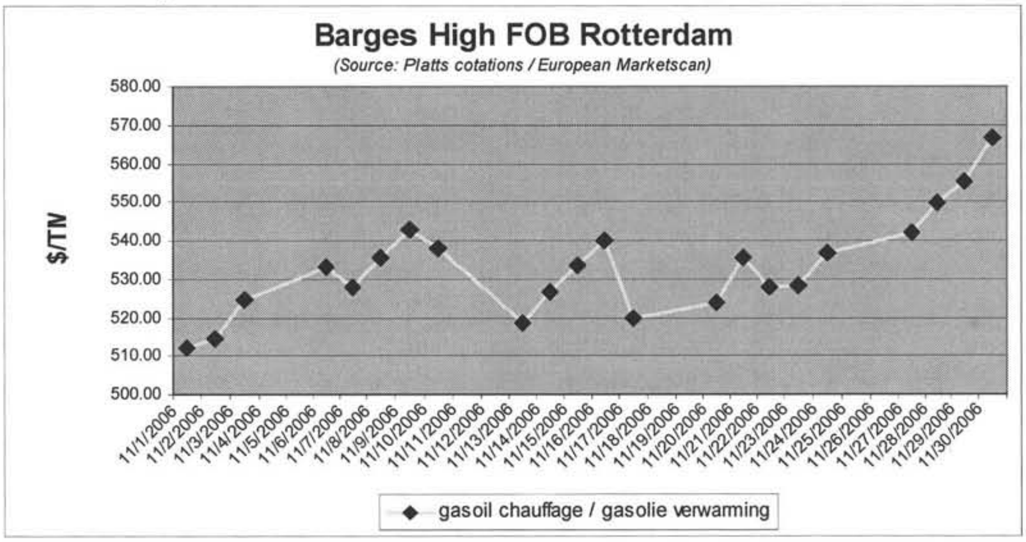
The heating oil is subject to the latest environmental regulations. Every year these regulations become more stringent with regard to sulphur content. The most up-to-date regulations can be requested from the DCMR, the Environmental Protection Agency for the region Rijnmond; the larger 'Port of Rotterdam'-area in the Netherlands.

1.3 Market information

Heating oil is not much used for heating in the Netherlands anymore. The majority of the heating oil produced in the Netherlands is exported to neighbouring countries such as Belgium and Germany. The United States of America also have a very high consumption of heating oil.

The market for heating oil is, as other refinery products, dependent on the crude price. But the heating oil market is also dependent on the demand of heating oil. In wintertime the demand for heating oil obviously increases, as do the prices.

The heating oil prices for November 2006 have been put in Figure 1.4. The prices mentioned are in dollar per ton.


Barges High FOB Rotterdam

(Source: Platts cotations / European Marketscan)

Figure 1.4: Heating oil prices from Rotterdam port.

1.4 Status of the process

The current process has been running for some time now. Projects for the GO-finer unit result from higher production rates and a misplaced feed point of the hydrocarbons to the fractionator. Now the cause of revamp of this unit is more stringent sulphur regulations. The sulphur content of the GO-finer Distillate should decrease to 50 ppm.

1.5 Available processes and preferred selection

Several process options have been found to, in one way or another, desulphurize the GO-finer feed to 50 ppm. In chapter 2.1 these options will be broadly explained. However a small overview of the most promising options is presented here.

1.5.1 Available processes

1. Intermediate H2S removal

To decrease the influence of H_2S inhibition in RX2 it could be useful to have H_2S removal between the 2nd and 3rd bed. A stream is send to a HPHS to remove the H_2S. Unfortunately this will also result in removal of H_2. The removal of H_2S will result in *a bigger H_2 recycle stream from the MEA unit.* As only the liquid is recycled from the HPHS, hydrogen partial pressure needs to be reinforced in RX2. This can only been done by the addition of extra H2. However this needs to be proved by simulations.

The H_2 throughput is not the only decision factor. The HPHS needed to perform the separation needs to be operated on a certain temperature (we assume 344 °C). To reach this temperature, the stream needs cooling. After separation the liquid stream needs heating (up to 405 °C) to be inserted at the right reaction temperature in RX2. *For this cooling and reheating we need a heat exchanger, a cooler and a heater (utilities not accounted for).*

2. Larger RX2

By replacing the RX2 with a bigger reactor, *the reaction time can be increased*, which will increase the desulphurisation rate. To achieve the requested sulphur content the reactor volume should be 900 m3. This is due to the high inhibition rate of the H_2S. Construction of this reactor will be very expensive. Steel-price and catalyst consumption)

3. Counter current flow in RX2

By using counter current flow in RX2, the reactor could be smaller. In counter current flow mode the fresh H_2 would contact the hardest to convert complex sulphur molecules first, at the part of the reactor where the H_2S concentration is large. By adding fresh H_2 the partial pressure of H_2S is reduced and the reaction rate increases. However *flooding* might occur in this flow type.

4. Semi counter current flow with RX3

By installing a reactor (RX3) in semi-counter current flow *directly* behind RX2 *no extra heating is necessary*. As the temperature of the liquid flow leaving RX2 is approximately 390 °C, this is an ideal inlet temperature for the liquid going in RX3. No additional heating will be required. The extra H_2 consumption will still have to be simulated, but it is expected that this would not be much. RX2 will need slight adjustments to provide a vapour and a liquid outlet stream. The reactor volume of RX3 is calculated to be 100 m3.

5. Co-current flow with use of current HPHS

To perform the least changes possible to the existing equipment, we could introduce the RX3 downstream of the HPHS. The RX3 is situated here, because the HPHS will already separate the vapour and liquid streams from the RX2. *Now RX2 will not need adjustment*. However, a lower temperature than the reaction temperature (400 °C) is required in the HPHS. This temperature is accounted for in the current heat system, but to achieve the reaction in RX3, the temperature of the (liquid) stream leaving the HPHS (345 °C) needs to be increased. *A heat exchanger needs to be installed.* The reactor volume of RX3 will be 100 m^3, the area necessary to perform the heating can be calculated once the utilities are known.

6. Fixed bed RX3 for Distillate stream

Installing a fixed bed (RX3) reactor for only the Distillate stream could be economically attractive, as the Distillate stream is smaller compared to the total stream leaving RX2. However, here we encounter other problems. The reactor needs to be purged with H_2. As there is no H_2 present in the Distillate stream, a fair amount of H_2 needs to be used to guarantee sufficient H_2 partial pressure. This additional H_2 will have to be recycled. This recycling will pull a *heavy load to the compressor*. As the Distillate stream leaves the fractionator the temperature of the stream is 45 °C. In order to have hydrogenation reactions in RX3 the temperature needs to be increased to approximately 400 °C. *A heat exchanger will have to be installed.* To have a satisfactory reaction in RX3 not only the temperature needs to be up to a certain point, *the pressure also needs to be increased tremendously*. The Distillate product is now leaving the system at 8.7 bar. This needs to be increased to at least 90 bar. A good pump will need to be installed to achieve this. After the reaction in RX3 the streams still need to be separated, *a HPHS or a distillation column needs to be installed.*

7. Reactive distillation

Although an economic evaluation proved that reactive distillation could be a very attractive choice, this option was not chosen as it is *not (yet) proven technology.* In literature research was found on reactive distillation for naphtha feeds. However, it was concluded that the naphtha set-up couldn't be a good representative with respect to the current reactive distillation feed-to-be.

1.5.2 Preferred selection

The final selection is done based on criteria described in 2.3.1. The concept chosen is the "Semi-counter current flow with RX3". The function of all equipment of the revamped GO-finer unit is described in 5.1. The block scheme of this concept is presented in Figure 1.5.

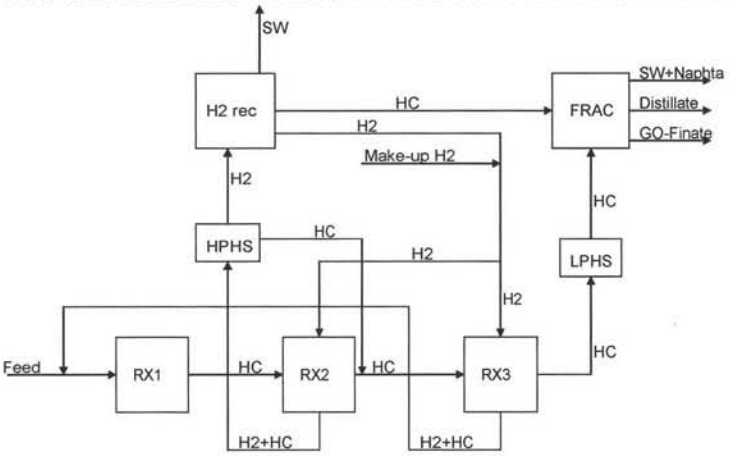


Figure 1.5: Concept chosen for the revamp of the GO-finer unit

An additional RX3 is installed in semi-counter current flow with RX2. For this purpose RX2 needs adjustment to the bottom-part of the reactor. The current HPHS will be used to separate the vapour effluent of RX2. A mayor part of the hydrocarbons present in the vapour stream are recycled as a liquid stream to RX3. The liquid effluent from RX3 is routed to the current LPHS. The vapour effluent is recycled to the reactor feed, where it is used as both reactant gas and to heat the feed. The vapour stream from the HPHS is treated in the H_2 recovery unit. This involves separation by a HPCS, treatment in a MEA unit and compressing it to operating pressure.

1.6 Availability of physical data

The physical data as represented in Table 3.2 were obtained from the handbook of chemistry and physics. Physical data for the many pseudo-components was obtained from several other references. From the component specification molecular weight could be calculated.

1.7 Patents

Several patents for the treatment of liquid sulphur-containing hydrocarbon feedstock are present. Most patents concentrate on the catalyst and catalyst preparation for this process. For example US patent 6531054 by Akzo Nobel (now Albemarle) and US patent 6444865, which is a Shell Oil Company patent. However some patents about processes and units for this application are known. A patent that describe these processes are US patent 5292428 (Davy McKee Ltd). No patents were found comprising the proposed process option.

2 Process options and selection.

In order to achieve the required deep desulphurization, multiple options are available. The use of new and more active catalysts is one of them. However, active catalysts often have difficulties with high concentrations H_2S, due to the inhibiting nature of the H_2S. As the feed of the GO-finer unit contains 30 000 ppm S, the inhibiting factor must be taken into account. So the use of only new and more active catalysts will not be sufficient, a new process needs to be developed.

2.1 Options for desulphurization

Optimization and changes in the current process in order to get lower sulphur content and a sufficient amount of Distillate stream can be done with one, or a combination of the following technologies:

1. Revamp of the current RX2.
2. Additional reactor for deep desulphurization of the total process stream.
3. Additional reactor for deep desulphurization of only the Distillate stream.
4. Reactive distillation column for deep desulphurization.
5. Separate desulphurization of light and heavy fractions of the feed of the GO-finer.

2.1.1 Revamp of the current RX2.

The new-generation catalysts will be able to perform deep desulphurization. However, the current catalyst in RX2 also performs mild hydro cracking. This increases the amount of Distillate and also helps desulphurizing the feed. If part of the catalyst in the second reactor is changed to a deep desulphurization catalyst it is expected that the amount of Distillate will decrease. It should be noted that the assignment is to make sufficient deeply desulphurized Distillate. If, with a new catalyst, still sufficient hydro cracking is achieved in the current RX2 reactor, revamp of the current reactor could be considered.

2.1.1.1 Larger RX2

To ensure sufficient hydro cracking, while performing desulphurization, one option is to replace RX2 with a larger reactor. By doing so, *the reaction time can be increased*, which will increase the desulphurization rate. The reaction time for hydrocracking is also increased, which will result in an increase of desulphurized Distillate.
To achieve the requested sulphur content *the reactor volume should be 900 m^3*. (Calculations can be found in 15.7.3) This is due to the high inhibition rate of the H_2S (see 0 for more about the inhibition of H_2S). As the reactor needs an inside layer of SS (because of the corrosive nature of sulphur) and an outside shell of CS, construction of this reactor will be very expensive. Furthermore, it will most probably not possible to place a reactor this big in the area provided for construction.

2.1.1.2 Intermediate H2S removal

RX2 can be split into two sections with intermediate H_2S removal by a HPHS. If the influence of H_2S inhibition in RX2 is decreased, the size of the revamped reactor could decrease as well (compared to the size mentioned in option 2.1.1.1). The size of the current reactor might even be big enough.
The first section is used for desulphurization, mild hydrocracking and denitrogenation. The second section is solely used for deep desulphurization. To decrease the inhibiting effect, H_2S will be removed halfway the second reactor. The process stream is retrieved between the 2nd and 3rd bed and send to a HPHS to remove the H_2S. Unfortunately this will also result in

removal of H_2. As only the liquid is recycled from the HPHS, hydrogen partial pressure needs to be reinforced in RX2. This can only been done by the addition of extra H_2. The removal of H_2S will thus result in *a bigger H_2 recycle stream from the MEA unit.*

The high H_2 throughput is not the drawback. The HPHS needed to perform the separation has to be operated on a certain temperature (344°C is assumed, as the current HPHS also operates at this temperature.). To reach this temperature, the stream needs cooling. After separation the liquid stream needs heating (up to 405 °C) to be inserted at the right reaction temperature in RX2. *For this cooling and reheating we need a heat exchanger, a cooler and a heater (Extra consumption of utilities are not taken into consideration at this point.).*

2.1.1.3 Counter-current flow in RX2

By using counter-current flow in RX2, the reactor could also be smaller in respect to option 2.1.1.1. In counter-current flow the fresh H_2 would contact the hardest to convert complex sulphur molecules first, at the part of the reactor where the H_2S concentration is large (inhibition). By adding fresh H_2 the partial pressure of H_2S is reduced and the reaction rate increases. In this way the inhibition of H_2S is accounted for.

However, as known for counter current flow reactors in general, *flooding might occur in the reactor.* It is possible to engineer the reactor in this way, that flooding will not occur, but this will result in *loss of operation freedom of the unit.* Since the unit has a variable feed operating this unit is almost not possible to operate.

2.1.2 An additional reactor for total process stream

The second general option would be to install an additional reactor (RX3) downstream of RX2. Taking the pressure profile throughout the whole GO-finer unit into account, it would be a convenient place for RX3 to either install it directly after RX2, or after the HPHS in the current operation. By installing the new RX3 here, the complete process stream will be treated. As the pressure is still high (91 bar) it would be ideal because high partial hydrogen pressures are needed for the hydrogenation / desulphurization reactions. For a representation of the flow scheme see Figure 2.1.

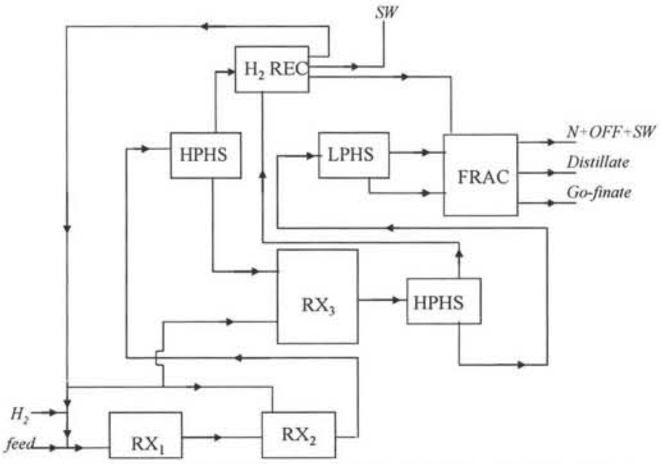


Figure 2.1: An additional deep desulphurisation reactor.

2.1.2.1 Additional Fixed bed reactor

A fixed bed reactor, as used for RX2 now, could be installed as RX3. This technology is proven and operating conditions are known, as the same catalyst present in RX2 will be used. The RX3 would be placed after the current HPHS, so the HPHS will already have separated the vapour and liquid streams from the RX2. This will minimize the inhibition effect of H_2S. An additional HPHS is installed between RX3 and the LPHS to prevent a high consumption of H_2. To prevent the H2 to be used as fuel gas, a recycle from the additional HPHS to the MEA unit will be installed. For this option RX2 will not need any adjustments.

However, the HPHS requires a lower temperature (344 °C) than the reaction temperature required in RX3 (400 °C) The temperature of the (liquid) stream leaving the first HPHS (344 °C) needs to be increased. *A heat exchanger will need to be installed.* The reactor volume of RX3 will be 100 m^3, (calculations in 15.7.3).

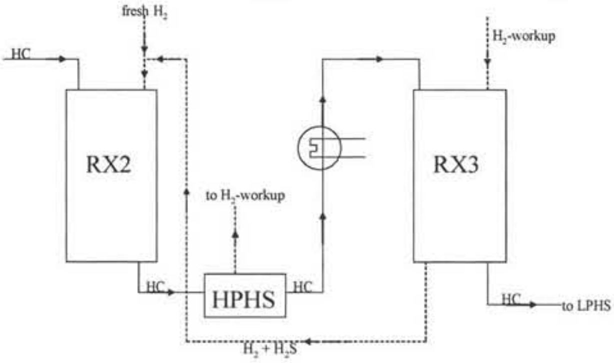


Figure 2.2: An additional fixed bed reactor in co-current mode

2.1.2.2 Reactive adsorption

For RX3 reactive adsorption with a catalyst and adsorbent can also be considered [5]. The adsorbent contains a catalyst, which promotes the reaction of H_2 with the sulphur containing components. The formed H_2S is subsequently adsorbed on to this adsorbent. Either continuous or periodic desorption of H_2S is needed. The periodic option means downtime of the unit. The continuous regeneration of the adsorbent can be chosen if sulphur content of the feed is higher. Continuous regeneration results in moving adsorbent particles. Attrition of the particles and energy needed for moving the particles have to be taken into account. The necessity of evaporating the feed for proper contact with the moving particles results in high temperature (> 400°C). The pressure needs to be high for reasonable reaction rates, but this will result in limited space velocities.

This option will require a high number of new equipment.

2.1.2.3 Extraction of the aromatic compounds

Another option is extraction of the aromatic compounds that contain sulphur. Extraction and separate treatment will result in smaller streams to treat. The aromatic compounds containing sulphur and especially the (substituted) benzothiophenes are difficult to desulphurize. A disadvantage is that the extraction *solvents for this process are not very selective.* This will result in either extracts with a lot of non sulphur containing components (so still a fairly large stream to process) or the extraction does not remove enough sulphur containing components to meet the specifications. Also, additional extraction and regeneration columns are needed which consume a lot of space.

2.1.2.4 Semi counter current flow with RX3

The additional reactor (RX3) can be installed in *semi counter current mode* of operation. For this option vapour and liquid streams need to be separated and follow different flow schemes. The fresh H_2 enters the RX3 and the vapour stream leaving RX3 is sent to RX2. This vapour contains H_2S, H_2 and some light fractions. In this way the inhibition of H_2S is limited, because the fresh H_2 is sent to RX3 first, where deep desulphurization is needed. In RX2 the sulphur content is already high; the reaction will take place even in the presence of contaminated H_2 (with H_2S). The H_2 recycle will not exceed the current recycle by a lot, which can be considered an advantage.

By installing a reactor (RX3) in semi-counter current flow *directly* behind RX2 *no extra heating is necessary*. (as shown in Figure 2.3) As the temperature of the liquid flow leaving RX2 is approximately 390 °C, this is an ideal inlet temperature for the liquid going in RX3. No additional heating will be required. RX2 will need slight adjustments to provide a vapour and a liquid outlet stream. The reactor volume of RX3 is calculated to be 100 m^3.

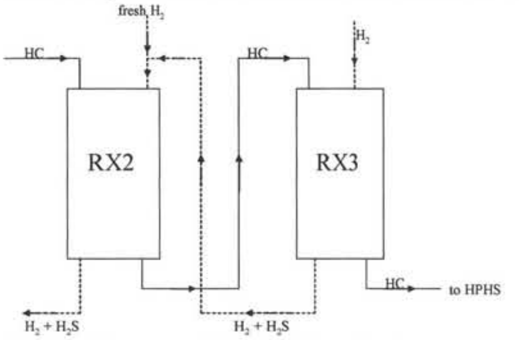


Figure 2.3: An additional fixed bed reactor in counter current mode

2.1.3 An additional reactor for Distillate

Since only the Distillate sulphur content is important, a reactor can be placed after the fractionator. Because only the Distillate stream is involved the reactor can be smaller. Figure 2.4 gives the flow sheet for this option.

A disadvantage of this option is that the pressure and temperature of the Distillate leaving the fractionator are too low. Compression costs and heating costs will be large, especially compression from 2.5 to 5 bar to at least 90 bar. An additional compressor is needed and also, separation of H_2S, H_2 and Distillate is needed.

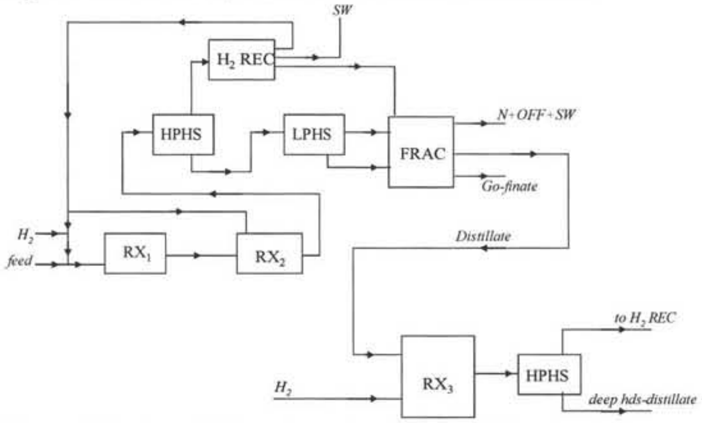


Figure 2.4: An additional reactor for Distillate stream

2.1.3.1 Enzymes for Distillate stream

An option for this reactor that does not need re-pressurizing and heating of the Distillate (process stream) is the use of *enzymes*. This can be done in two different ways, namely by using the micro-organisms (MOs) or by isolating the enzymes (which can be free or immobilized). MOs will form numerous by-products and they degrade the Distillate, therefore it is favourable to use enzymes (which are far more selective). The conditions are normally at ambient pressure and temperature and the enzymes are in an aqueous solution.

This condition immediately introduces a problem; the volumetric ratio of the organic and the aqueous phase. This will result in a *very big reactor*, which will result in *high investment costs*. It is estimated that the reactor will turn out to be 360 m^3. This will result in high investment costs. Enzymes are very expensive to produce, so a high amount of bio-catalyst (which is needed for the deep HDS) will be costly. Finally, it is relatively difficult to extract the enzymes from the process for reuse and to purify the treated Distillate stream. Extracting and purifying the enzymes from the organic product stream is a multi-step operation which will require *more units.*

Summarized, the use of enzymes is a nice idea because it can be done at ambient pressure and temperature, but the size of the reactor needed and the work up after the reaction is hard and very expensive [6].

2.1.4 Reactive distillation

The reactive distillation has been investigated for naphtha streams [5] with 250-300 ppm S, so to make sure it will work similar sulphur content is prudent. A better catalyst for the second reactor will be reasonable. This ensures that the stream leaving the second reactor is desulphurized as much as possible. The separation of H_2S is performed simultaneously with the desulphurization. The catalyst bed is constantly wetted, thus cleaned and the operation is conducted counter-currently. In both the top and bottom sections of the column normal trays can be placed to ensure good separation. The pressure in the reactive distillation should be around 20 bar. A block scheme is shown in Figure 2.5.

Moreover, the current fractionation column would have to be replaced by a new reactive distillation column.

Although an economic evaluation proved that reactive distillation could be a very attractive choice, this option was not chosen as it is *not (yet) proven technology.* In literature research was found on reactive distillation for naphtha feeds; however it was concluded that the naphtha set-up couldn't be a good representative with respect to the current reactive distillation feed-to-be.

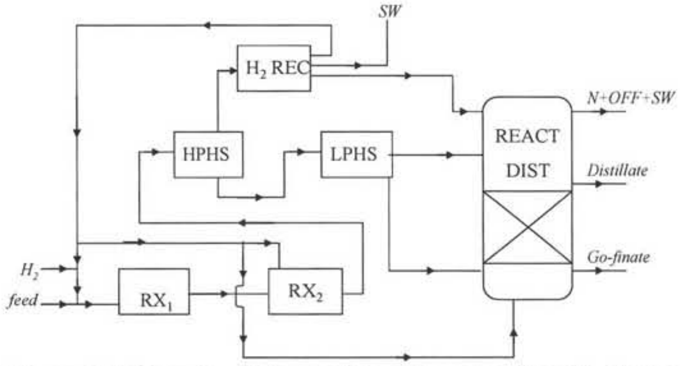


Figure 2.5: Deep desulphurisation with a reactive distillation column

2.1.5 Separation of light and heavy fractions before entering RX2

In the literature [8] it is recommended that light and heavy fractions should be treated separately due to their different reactivity's. A flash vessel between the guard reactor and the second reactor can be used to separate the light and heavy fractions, see Figure 2.6. It is chosen to prevent contamination with metals (during downtime of the guard reactor) of the two smaller beds in the second reactor through the placement of a second parallel guard reactor.

After the second reactor both treated process streams are sent to a new HPHS to separate the H_2S and H_2 from the process stream before deep desulphurization in the third new reactor takes place.

However, this is not a very useful option because there is only a small part of light fraction. Moreover, the light and heavy fractions from the Flexicoker are first mixed and filtered sent to the guard reactor and split again. Furthermore, the second reactor is also used for mild hydrocracking, so the production of sufficient Distillate is jeopardized.

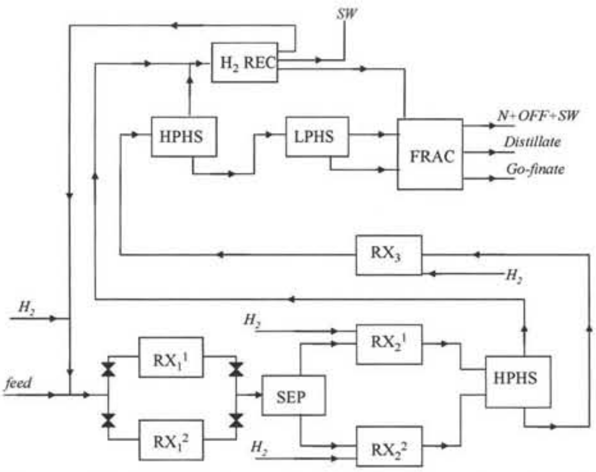


Figure 2.6: Separation of light and heavy fractions before HDS

2.2 Additional revamp options

When the GO-finer unit is to be revamped, it should be investigated if a new parallel placed guard reactor is attractive. A parallel guard reactor will provide more protection for the second reactor during down time of the current guard reactor. This will enhance the lifetime of the catalyst in the second reactor.

If the second reactor is not revamped and left as mild hydro cracker, a third deep desulphurization reactor with an active and probably more expensive catalyst is necessary. The life time of this catalyst should be as long as possible. In the case the life time of the catalyst is longer then one and a half years, it is rewarding if the second reactor has a longer on-stream time as well. This can be accomplished with a parallel guard reactor. A block scheme of this option can be found in Figure 2.7.

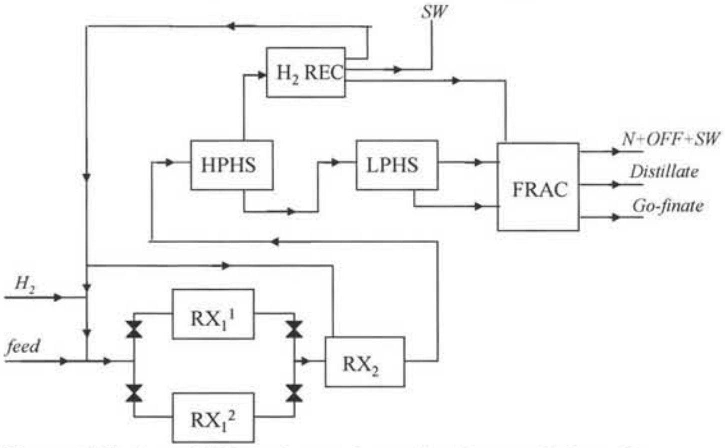


Figure 2.7: An additional guard reactor in parallel mode

The costs for the additional guard reactor can be summed. The following assumptions are made:

- The height of the reactor is 3.5, the diameter is 2.5 meter, the steel has a volume of 0.31 m^3. With a (average) density of 8000 kg/m^3 this results in 2500 kg steel.
- The steel price is €8.00 per kg SS .
- The extra consumption of 6 catalyst beds in 15 year, with a volume of 17 m^3.
- Catalyst has a density of 700 kg/m^3 and costs €15.00 per kg.

Table 2.1: Catalyst and equipment costs

Costs	Euro
Equipment	1 9750.00
Catalyst	1 071 000.00
Total	1 090 750.00

As the profit of the GO-finer unit per hour is € 1164.00, this is also the loss of the GO-finer during down time. Now calculating the number of weeks the GO-finer unit should be down to have losses as much as the costs for an extra Guard reactor, this would result in *40 weeks in 15 years*. As the GO-finer now experiences only 10 weeks down time in 15 years, this option *wouldn't be profitable*

2.3 Decision for the revamp of the GO-finer unit

As multiple options have been proposed in the previous sections, only one option should be chosen for the final design.

2.3.1 Decision criteria

From the options proposed in Chapter 2.1 a sound decision needs to be made which option to choose. To make this decision, a number of selection criteria were formulated. The criteria of selection are:

- Number of units;
- H_2 consumption;
- Feasibility;
- Production costs.

These selection criteria were chosen because of the following reasoning:

- Number of units; although there is space available in the GO-finer unit to install new units, this area is not too big. Attempts need to be made to install as less as possible units. Lesser units will also result in lower investment costs and higher controllability.
- H_2 consumption; as H_2 is consumed by the process, it is of importance to minimize this consumption. It is also important to have low H_2 consumption as the compressor for the recycle has a limited capacity. If this capacity is reached, H_2 will be purged, which will result in a loss of H_2
- Feasibility; some of the mentioned options are not yet proven technology, or it is (not yet) proven that the sulphur specification can be met. Research on the applicability of these options to the GO-finer unit will need to be done. Until then, it is a high risk to introduce these options to the unit.
- Production costs; a basic economic evaluation of an option often starts at the production costs. If the costs of these non-recoverable consumption goods, like catalysts, H_2, sorbents and enzymes are already high, it is unlikely to have a good economic evaluation.

2.3.2 Decision

Based on the above-mentioned decision criteria an overview can be made, see Table 2.2.

Table 2.2: Decision on the design options

	Revamp RX2			RX3			
	Larger RX2	H2S removal	Counter Current flow	RX3 Co-current + HPHS	Reactive adsorption	Extraction	RX3 Semi-counter current
Feasibility			XXX		XXX	XXX	
Production costs	XXX				X		
H2 consumption	XX	XX		X			
Number of units		XX		X	X	XX	X

	RX3 Distillate			
	Fixed bed	Enzymes	Reactive Distillation	Separation of fractions
Feasibility		XXX	XXX	XXX
Production costs		X		
H2 consumption				
Number of units	XXX	XXX		XX

As shown in the above table, all options have drawbacks. However, the options that have triple X are the most unfavourable. The options having double X are better, and the options only having a single X are even better. From the table it shows that two options don't have double or triple X's. These options are the "RX3 Co-current +HPHS" and the "RX3 Semi-counter current". However the "RX3 Semi-counter current" option only has one X. Therefore, this option will be chosen as the design option.

2.3.3 Chosen concept

After considering all revamp options for the GO-finer (see 2.1 and 2.2), a choice is made. In Figure 2.8 the block diagram of the chosen concept is shown. Heat exchanger systems and pumps are taken out of consideration. These will be discussed in 5.1.

- The feed is mixed with H_2. In RX1 the metals and other contaminants are removed. The stream is than transported to RX2, where desulphurization and mild hydrocracking takes place as in the current operation.
- The bottom of the RX2 is adjusted to be able to have a vapour and a liquid outlet. A tray is installed that will be able to catch the liquid. A pipe will be installed to deplete the vapour.
- The vapour stream from RX2 is send to a HPHS to separate the (condensable) hydrocarbons present in the vapour stream. The vapour stream is routed to the H_2 work-up.
- In the H_2 workup, H_2S is removed. The light hydrocarbon fractions go to the fractionator and the treat-gas stream (containing H_2 and C1-C4 gasses) is recycled.
- The condensed hydrocarbons are mixed with the liquid stream from RX2 and send to RX3.
- In RX3 the final desulphurisation takes place, reaching a sulphur content of 225 ppm. In the RX3 the vapour and liquid stream are separated (as in RX2).
- The vapour stream contains H_2, which will be routed to either RX2 or to the feed where it is mixed.
- The liquid stream is sent to the LPHS, from where the heavy and light fractions are separated. Both fractions are then routed to the fractionator, where they are inserted at different heights.

- At the bottom of the fractionator, steam is added. The fractionator separates all the compounds in a GO-Finate stream, Distillate stream, Sour Water, Naphtha and Offgas stream.

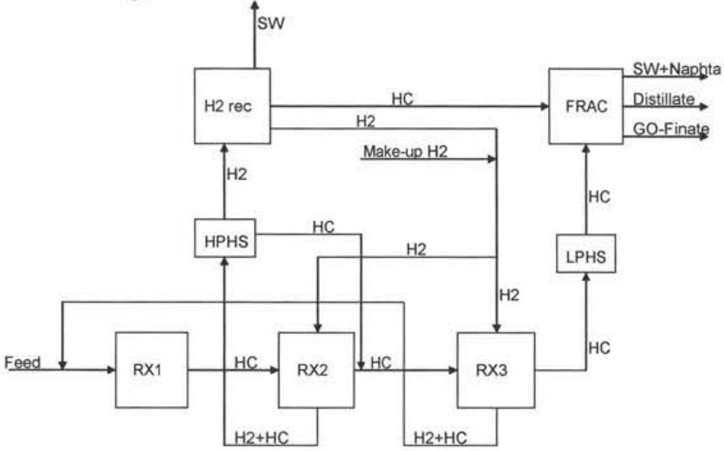


Figure 2.8: Concept chosen for the revamp of the GO-finer unit

3 Basis of Design

The Basis of Design provides all key data for the design is tabulated and provided with background information. Items such as feedstock, products, wastes, utilities, specific equipment, plant location, costs etc are covered. The Basis of Design normally is a separate document with all information. For this report, the BoD is part of a whole, so information will be brief and references will be made to other chapters.

3.1 Description of the design

The GO-finer unit is part of the ExxonMobil refinery in Rotterdam. The focus of the refinery is to produce middle distillates (Diesel and Heating oil) from crude oil.

The vacuum Distillate from the crude distillation tower is sent to the Flexicoker, where it is converted into fuel gas, naphtha and coker gas oil (LKGO and HKGO). The KGO streams have a high metal, sulphur and poly-aromatic content and will be treated by a hydro treating unit: the GO-finer. The main product streams are the GO-finer Distillate, with a maximum S-content of 2500 ppm, and the GO-Finate, with at maximum 10 000 ppm S. The Distillate is blended into heating oil and the GO-Finate serves as hydrocracker feedstock.

Due to more stringent regulations in future the sulphur content in the Distillate stream needs to be reduced to 50 ppm. The design is based on the request of ExxonMobil to be able to produce this Distillate in the future. Modifications and additions to the current GO-finer unit are in the scope of this design.

3.1.1 Design background

The current GO-finer unit has an intense integration of mass and heat streams. A simplified block scheme is shown in Figure 3.1. The feed is mixed with hydrogen and sent to the reactor section. This section consists of two separate reactors, RX1 and RX2. In RX1 the metals are removed. In RX2 hydrodesulphurization and some mild hydrocracking takes place. The reactor effluent is sent to a high pressure and hot separator (HPHS), where most of the formed H_2S, some hydrocarbons and excess H_2 are removed. This stream is then treated in a high pressure cold separator (HPCS). Here the gas is separated for recycle. The hydrocarbons are returned to the fractionator and sour water is sent to a SW-stripper. The recycle gas is sent to a MEA scrubber, which removes any residual impurities (mainly H_2S). The treated H_2 is now recycled to RX1 and RX2. After the HPHS the liquid hydrocarbon stream is sent to a low pressure hot separator (LPHS), which separates heavy and light fractions, to optimize the subsequent fractionation.

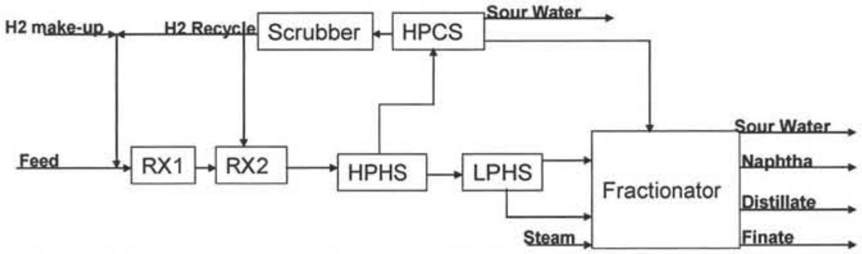


Figure 3.1: Block scheme of current GO-finer operations

3.1.2 What will (not) be done

In this design we will not attempt to optimize the Flexicoker operations. It is assumed that the feed stream is constant in composition and that the utilities needed are available. The treatment of the extra waste streams will not be considered. The design will focus on reduction of the sulphur content and not the nitrogen content or the poly-aromats. This might be affected, but it will not be the main objective.

A process alternative will be proposed that can produce < 50 ppm sulphur in the GO-finer Distillate stream. For this we will look at different options. These can include different reactor configurations or operations, new catalysts or new techniques available like extraction or reactions with enzymes.

In varying detail the thermodynamics and kinetics for the chosen option will be given, as well as the process streams and mass balances and some block schemes. Basic assumptions will be given and the economic margin will be calculated.

3.2 Process definition:

3.2.1 Process concepts chosen

In order to achieve the required deep desulphurization, multiple options are available. The use of new and more active catalysts is one of them. However, multiple process alternatives might also do the trick. The alternatives are summarized below, but are explained in more detail in 2.

1. Revamp of the current RX2.
2. Additional reactor for deep desulphurization of the total process stream.
3. Additional reactor for deep desulphurization of only the Distillate stream.
4. Reactive distillation column for deep desulphurization.
5. Separate desulphurization of light and heavy fractions of the feed of the GO-finer.
6. Additional guard reactor

The process chosen is option 2. The reasoning behind this choice is explained in more detail in 2. A block-scheme is shown in Figure 3.3.

- The feed is mixed with H_2. In RX1 the metals and other contaminants are removed. The stream is than transported to RX2, where desulphurization and mild hydrocracking takes place as in the current operation.
- The bottom of the RX2 is adjusted to be able to have a vapour and a liquid outlet. A tray is installed that will be able to catch the liquid. A pipe will be installed to deplete the vapour.
- The vapour stream from RX2 is send to a HPHS to separate the (condensable) hydrocarbons present in the vapour stream. The vapour stream is routed to the H_2 work-up.
- In the H_2 workup, H_2S is removed. The light hydrocarbon fractions go to the fractionator and the treat-gas stream (containing H_2 and C1-C4 gasses) is recycled.
- The condensed hydrocarbons are mixed with the liquid stream from RX2 and send to RX3.
- In RX3 the final desulphurisation takes place, reaching a sulphur content of 225 ppm. In the RX3 the vapour and liquid stream are separated (as in RX2).
- The vapour stream contains H_2, which will be routed to either RX2 or to the feed where it is mixed.

- The liquid stream is sent to the LPHS, from where the heavy and light fractions are separated. Both fractions are then routed to the fractionator, where they are inserted at different heights.
- At the bottom of the fractionator, steam is added. The fractionator separates all the compounds in a GO-Finate stream, Distillate stream, Sour Water, Naphtha and Offgas stream.

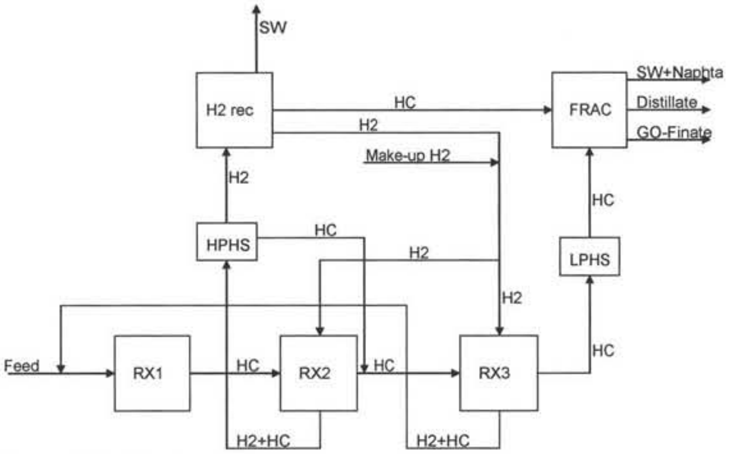


Figure 3.2: Block scheme of process option chosen

The specification of the in- and outgoing streams is presented with the battery limit, Table 3.3.

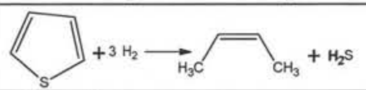
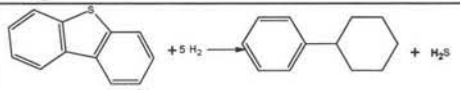
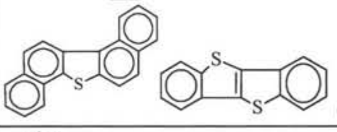
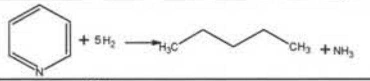
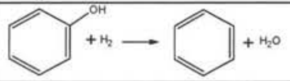
3.3 Thermodynamic Properties & Reaction Kinetics

As there are multiple components in the GO-Finer unit feed, thermodynamics and reaction kinetics are hard to model. From various literature sources some basic reaction pathways have been proposed, see 15.1. Mild hydrocracking was also taken into account.

3.3.1 Reactions

The feed stream contains a variety of sulphur compounds. A summary of the most important ones is given in Table 3.1. Also the heats of reaction of some compounds are shown.

Table 3.1: Summary of sulphur containing compounds in gas oil [18]

Compound	Example reaction	ΔH^0_{298}(kJ/mol)
Mercaptans	$RSH + H_2 \rightarrow RH + H_2S$	-72 ($R=CH_3$)
Thiophenes		-147
Benzothiophenes and substituted benzothiophenes	  (and variations of both)	-225
Pyridines		-333
Phenols		-62

A complete list of the sulphur containing components is given in 15.1. Dibenzothiophene (DBT) and 4,6-dimethyldibenzothiophenes (4,6-DMDBT) are the compounds most difficult to desulphurize. They are used as model compounds. They undergo desulphurization via two pathways:

1 Direct desulphurization (DDS), which leads to the formation of biphenyls;
2 Hydrogenation (HYD) yielding tetrahydro- and hexahydro-intermediates followed by desulphurization to cyclohexylbenzenes and bicyclohexyls.

A schematic of these reactions is shown in Figure 3.3 [10]:

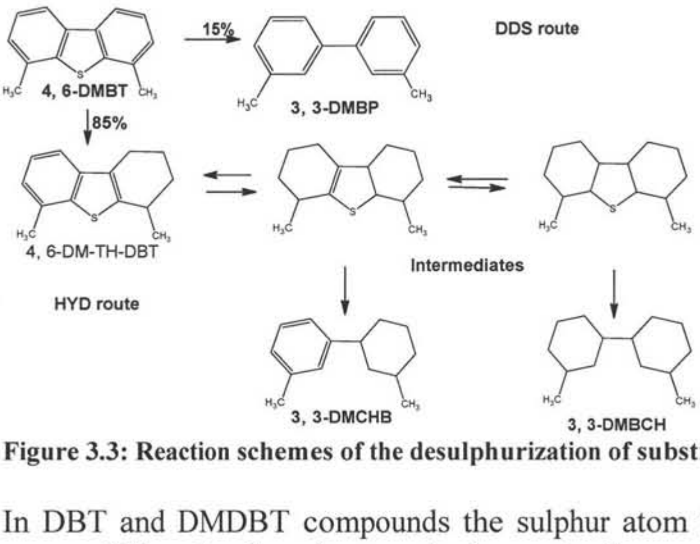


Figure 3.3: Reaction schemes of the desulphurization of substituted benzothiophenes

In DBT and DMDBT compounds the sulphur atom is sterically hindered by the two alkyl groups. When the phenyl-groups hydrogenate, they can take on other conformations and more easy to desulphurize. Due to the strong reducing environment in the reactor, most phenyl groups will hydrogenate and thus the HYD route will be more favourable.

3.3.2 Reactivity

In various studies done to compare the reactivity's of the different compounds it was shown that the alkyl substituted DBT's are most unreactive. Moreover, their desulphurization is retarded by the presence of poly-aromatic compounds, because they occupy the catalyst for hydrogenation. Basic organic nitrogen compounds are also competitive inhibitors, just like the H_2S formed.

The rate constants of all components could be estimated in computer simulations, since the composition of the in- and outgoing streams of the reactor are known in detail. There are about 26 reactions that include several steps.

To model the desulphurisation reactivity a general Langmuir-Hinselwood type of rate equation can be used and is given in Equation 3-1.

$$r = \frac{k\ c_{org\ S}^{2} c_{H_2}}{1 + Kc_{H_2S} + Kc_{.....}}$$

Equation 3-1

This equation can be rewritten when partial pressures are known, Equation 3-2.

$$r = \frac{kK_{DBT}P_{DBT}}{\left(1 + K_{DBT}P_{DBT} + K_{H_2S}P_{H_2S}\right)}$$

Equation 3-2

k = rate constant
K= adsorption constant

C_{orgS}= concentration of sulphur-containing compounds

As the different types of sulphur containing components react at very different rates, a classification system has been proposed that groups components with similar reaction behaviour (hydrogenation, desulphurization, etc) and similar reactivity. This reduces the number of rate constants and makes calculations easier. This classification system is given in 15.1.

3.3.3 Thermodynamics

As can be seen from the heats of reaction in Table 3.1 all reactions are exothermic. The equilibrium lies to the desulphurized products at the temperatures used (~410 ^{0}C), but the rate at which these equilibria are achieved is different. The problem lies in the reactivities as explained in the previous section. Hydrotreating of heavy fractions requires high temperatures and high hydrogen partial pressures compared to hydrotreating of light fractions.

In the selection of the thermodynamic model it was considered that ideality can only be assumed at pressures lower than 10 bar. An equation of state was chosen: for the gas phase it was decided to be Redlich-Kwong or Peng-Robinson. For the liquid phase the UNIQUAC method was chosen.

Accurate data on heat capacities and enthalpies are provided by the principals. The only important parameters that will be estimated are the rate constants.

3.3.4 Catalysts

Because the most difficult molecules desulphurize via the HYD route, a catalyst is needed that promotes hydrogenation as well as desulphurization. Noble metals can best be used in a second reactor of a two-stage hydrotreater, where the formed H_2S is removed before it enters the reactor and the sulphur content is low enough for the metals to maintain enough activity.

However in this design a conventional metal sulphide catalyst (NiMO) is chosen, because noble metals are very expensive. Moreover, good results can also be obtained with this catalyst.

3.4 List of Pure Component Properties

To have an impression which components are present in the GO-finer unit, an overview is given in Table 3.2. Technological data is (as known) represented as well as the medical data.

Table 3.2: List of pure component properties.

Pure Component Properties									
Component Name		Technological Data					Medical Data		Notes
Design	Systematic	Formula	Mol Weight g/mol	Boiling Point C	Melting Point C	Density of Liquid kg/m3	MAC Value mg/m3	LD50 g	
H2O	Water	H2O	18,02	100,00	0,00	0.99821 (1)			(1) @ 20C
H2	Hydrogen	H2	2,01594	-252,87	-259,34	0.082 (2)			(2) g/L
C1	Methane	CH4	16,04	-161,50	-182,40	0.4228 (3)			(3) @-162 C
C2	Ethane	C2H6	30,07	-88,60	-182,80	0.5446 (4)			(4) @ -89 C
H2S	Hydrogensulfide	H2S	34,08	-59,55	-85,50	1.393 (2)	15		
NH3	Ammonia	NH3	17,03	-33,33	-77,74	0.6996 (2)	14		
C3	Propane	C3H8	44,1	-42,10	-187,60	0.493 (5)			(5) @ 25 C
IC4	Isobutane	C4H10	58,12	55,20	-108,60	0.7405 (1)			
BUTENE	1-Butene	C4H8	56,11	-6,20	-185,30	0.588 (5)			
NC4	Butane	C4H10	58,12	-0,50	-138,20	0.573 (5)	1430		
IC5	2-methyl-Butane	C5H12	72,15	27,80	-159,90	0.6201 (1)			
PENTENE	1-Pentene	C5H10	70,13	29,90	-165,20	0.6405 (1)			
NC5	Pentane	C5H12	72,15	36,00	-129,70	0.6262 (1)	1800		
CYCLOPENTANE	Cyclopentane	C5H10	70,13	49,30	-93,80	0.7457 (1)			
ISOHEXANE	2-methyl-Pentane	C6H14	86,18	60,20	-153,70	0.650 (5)	720		
HEXENE	1-Hexene	C6H12	84,16	63,40	-139,70	0.6731 (1)			
NC6	Hexane	C6H14	86,18	68,70	-95,30	0.6548 (5)	90		
BENZENE	Benzene	C6H6	78,11	80,00	5,50	0.8765 (1)	3,25		
CYCLOHEXANE	Cyclohexane	C6H12	84,16	80,73	6,59	0.7739 (5)	875		
MEA	Mono-ethanolamine	C2H7NO	61,08	171,00	10,50	1.0180 (1)	2,5		
CO2	Carbon dioxide	CO2	44,01	-78.5 (6)	-56.57 (7)	0.720 (5)	9000		(6) @1 atm
PfxxxAxxdxxx			75						(7) @5.11 atm
177+			291,57						

3.5 Basic Assumptions

In this paragraph the current situation is presented. This is the starting point of the design.

3.5.1 Plant capacity and Location

The GO-finer is part of the ExxonMobil refinery situated in Rotterdam. The basic feedstock for the Go-finer is the heavy gas oil from the Flexicoker. These gas oils have relatively high sulphur content.

The main products of the GO-finer are the Distillate and the GO-Finate. The Distillate is to be blended to form heating oil and the GO-Finate is further processed in a hydrocracker. The plant produces 78 t/hr Distillate, with 2000 ppm S (end of run) and 54 t/hr GO-Finate containing 10 000 ppm S (end of run).

3.5.2 Battery Limit

The battery limit describes the streams going in and out the GO-finer unit. The feed streams are exit streams from the Flexicoker. The treat-gas feed does not have a variable composition but the rate can be changed. It is assumed that sour water can be treated no matter what the composition is.

The side streams from the fractionator are read of mass balances provided by the principles.

Concerning prices of products the following can be said:

Value of lowering Distillate sulphur:

- from ~ 1000 ppm to 50 ppm: + 15 $/t Distillate
- from ~ 1000 ppm to 10 ppm: + 20 $/t Distillate

By changing the operations, the GO-Finate may change as well. However changing the sulphur content does not have any value. Changing the density of the Finate from e.g. 960 kg/m^3 to 950 kg/m^3 is worth 10 $/t GO-Finate.

The Distillate is 60 $/t more valuable than the GO-Finate. Naphtha is 30 $/t more valuable than the Distillate. The price of the current catalyst is 15 €/kg.

These values are represented in Table 3.3

Table 3.3: Summary of in- and outgoing streams/substances passing the battery limit

Stream:		**112 (Feed)**	**135 (treatgas feed)**		**173 (Off gas to flexocoker)**		**172 (SW from fractionator)**		**177 (Naphtha product)**		**163 (Distillate product)**		**169 (GO-finate product)**		**153 (SW from scrubber)**		**141 Stripping steam to frac.**	
		Specification																
Comp	**Unit**	**C**	**C**	**D**	**C**	**D**	**C**	**D**	**C**	**D**	**C**	**D**	**C**	**D**	**C**	**D**	**C**	**D**
Hydrocarbons/aromatics	wt%	100	43 (4)	(1)	79 (4)	(1)	(3)	(3)	98 (4)	(1)	99 (4)	(1)	99 (4)	(1)	(3)	(1)	0	0
Sulphur (total)	ppm	30000	(3)	(3)	(2)	(1)	(2)	(1)	(3)	(3)	50	<50	2500	(1)	0	(1)	0	0
Nitrogen NH_3	ppm kg/hr	3000	(3)	(3)	(2)	(1)	12	(1)	(3)	(3)	1100	(1)	2500	(1)	258	(1)	0 0	0
H_2S	kg/hr	0	(3)	(3)	623	(1)	27	(1)	(3)	(3)	(3)	(3)	(3)	(3)	515	(1)	0	0
H_2O	kg/hr	0	32	32	103	(1)	6816	(1)	(3)	(3)	(3)	(3)	49	(1)	9998	(1)	60000	(1)
H_2	kg/hr	0	2569	2569	152	(1)											0	0
Rate	kg/hr	140 000	4548	(1)	4300	(1)	6856	(1)	3000	(1)	78000	78000	54000	54000	10775	(1)	60000	(1)
Process Conditions and Price																		
Temperature	^{0}C	310	60		41.3		41.3		47		45		90		46		154	(1)
Pressure	Bar	110	120		2.6		2.6		6.6		8.7		6.6		88.6		5.4	(1)
Phase	V/L/S	L	V		V		L		L		L		L		L		V	V
Price (5)	$/ton		1500						30		1	15	1/60	10/60				

Additional information:
C=Current
D=Design
(1) not yet available, depends on process simulation and mass balances
(2) not available from principals/to be negotiated with principals
(3) negligible
(4) approximate values
(5) prices relative to distillate at 1000 ppm

3.6 Economic Margin

In chapter 11 the economic evaluation of the project is performed. The main conclusions of it can be found in Table 3.4.

Table 3.4: Major economic parameters of the new design of the GO-finer.

Economic parameter	Unit	Value
Investment Costs	k$	$2 \cdot 10^3$
Annual Operating Costs	k$/yr	$105 \cdot 10^3$
Production Costs	$/kg Distillate	0.14
Total Annual Income	k$/yr	$11 \cdot 10^3$
"Net Annual Cash-Flow"	k$/yr	$-94 \cdot 10^3$

All economic parameters are additional costs and income in comparison with the current process (except the investment costs).
The investment costs are low in comparison with the annual operating costs. The annual production costs are high because of the hydrogen consumption (6 t/h more H_2 than current operation). Because of the high annual production costs, the "net annual cash-flow" is negative. This means that the project will cost money each year instead of becoming profitable after some time. In fact it will never be profitable.
The goal of the feasibility study is the reduction of the sulphur content of the Distillate stream. The reduction is required due to future legislation. Those adaptations in processes usually cost money instead of making profit out of it. But in order to make the process economical attractive, the annual operating costs have to be further decreased (which means that the hydrogen consumption has to be decreased).

4 Thermodynamic Properties & Reaction Kinetics.

When discussing thermodynamic properties and kinetics there are several points to keep in mind. The sequence of reactions that occur in the current reactor is very complicated and almost impossible to model. However an attempt is made to model these reactions from data provided by the principle on stream compositions, see 15.1 and 15.1.2. From various literature sources some basic reaction pathways have been proposed, see 15.1. These have indeed been observed in the scheme from 15.1.2. Mild hydrocracking has also been taken into account.

4.1 Reactions

The feed stream contains a variety of sulphur compounds. A summary of the most important ones is given in Table 3.1. Also the heats of reaction of some compounds are shown. A complete list of the sulphur containing components is given in 15.1. The mercaptans are the easiest to desulphurize. The sulphur atom is easy accessible and absorption on a catalyst site is not difficult. The same can be said for thiophene, phenol and pyridine.

Dibenzothiophene (DBT) and 4,6-dimethyldibenzothiophenes (4,6-DMDBT) are the most difficult compounds to desulphurize. They are, therefore, often used as model compounds. They undergo desulphurization via two pathways:

1 Direct desulphurization (DDS), which leads to the formation of biphenyls;
2 Hydrogenation (HYD) yielding tetrahydro- and hexahydro-intermediates followed by desulphurization to cyclohexylbenzenes and bicyclohexyls.

A schematic of these reactions is shown in Figure 3.3 [10]:

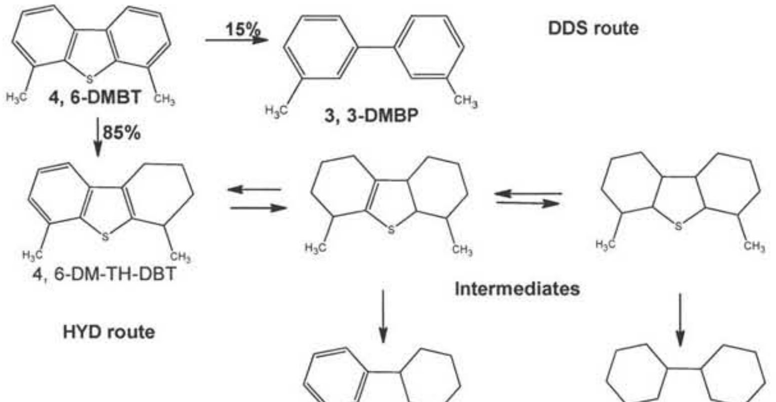
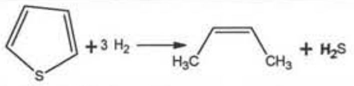
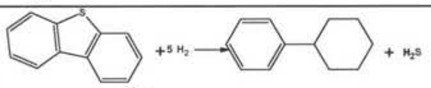
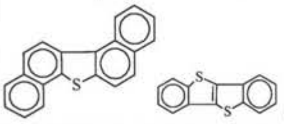
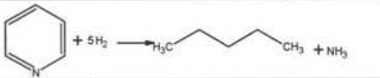
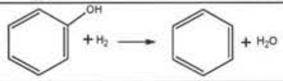


Figure 4.1: Reaction schemes of the desulphurization of substituted benzothiophenes

The percentages given are indications. The difficulty with these DBT and DMDBT compounds is that the sulphur atom is sterically hindered by the two alkyl groups. The phenyl-groups are flat. This makes the sulphur atom hard to reach. When the phenyl-groups hydrogenate, they can take on other conformations. This makes the sulphur atom more accessible. This contributes to the fact that these compounds are mostly converted via the HYD route. In contrast to this, benzothiophenes convert mostly via the DDS route, see also Table 4.1 for more information on this reaction. Due to the strong reducing environment in the reactor, most phenyl groups will hydrogenate and thus the HYD route will be more favourable. When the reaction scheme from 15.1 was composed this was indeed observed.

Table 4.1: Summary of sulphur containing compounds in gas oil [18]

Compound	Example reaction	ΔH^0_{298}(kJ/mol)
Mercaptans	$RSH + H_2 \rightarrow RH + H_2S$	-72 ($R=CH_3$)
Thiophenes		-147
Benzothiophenes and substituted benzothiophenes	  (and variations of both)	-225
Pyridines		-333
Phenols		-62

4.2 Reactivity

In various studies done to compare the reactivity's of the different compounds it was shown that the alkyl substituted DBT's are most unreactive. Moreover, their desulphurization is retarded by the presence of polyaromatic compounds, because they occupy the catalyst for hydrogenation. Basic organic nitrogen compounds are also competitive inhibitors, just like the H_2S formed.

The light fractions, mercaptans and thiophenes, react very fast. After this the reaction rate decreases rapidly, because the H_2S concentration has increased causing a high inhibition.

The specific kinetics of all components involved is not known. Some rate-constants can be found in literature, but they are usually measured for pure components. The inhibition effects are then not accounted for. Secondly they are measured at different reaction conditions. It is known that rate constants have a strong dependence on the temperature and can therefore not easily be extrapolated [9].

This makes it difficult to estimate the desulphurization efficiency of the process option chosen. The rate constants of all components could be estimated in computer simulations, since the composition of the in- and outgoing streams of the reactor are known in detail. There are about 26 reactions that include several steps. Since each step has its own rate constant, these calculations become very cumbersome, very fast.

One could group all sulphur-containing molecules together as if one reaction takes place. A general stoichiometric reaction is proposed [11]:

$$0 = \nu_A \mathrm{orgS} + \nu_B H_2 + \nu_C \mathrm{org} + \nu_D H_2S$$

The inhibition effects are taken into account with the stoichiometric constants by assuming $\nu_A=-1$, $\nu_B=-4$ and $\nu_C=\nu_D=1$.

From literature it [11]has been proposed that the apparent reaction order is now around second order. It is proposed to even be closer to 2.2.

This is the result of the lumping of several first-order reactions and the conversion of different sulphur compounds.

A general Langmuir-Hinselwood type of rate equation can be used and is given in Equation 3-1.

$$r = \frac{k\ c^2_{org\ S} c_{H_2}}{1 + Kc_{H_2S} + Kc_{.....}}$$

Equation 4-1

This equation can be rewritten when partial pressures are known, Equation 3-2.

$$r = \frac{kK_{DBT}P_{DBT}}{\left(1 + K_{DBT}P_{DBT} + K_{H_2S}P_{H_2S}\right)}$$

equation 4-2

k= rate constant
K= adsorption constant
C_{orgS}= concentration of sulphur-containing compounds

When the inhibition effects of nitrogen and aromatics are to be taken into account, the denominator has to be corrected accordingly. With this equation the catalyst volume needed can be determined and also the composition of the desulphurized stream calculated.
The hydrogen concentration could be assumed constant, since the quench provides enough hydrogen to make up for the reacted hydrogen. This method would however not yield a sufficient accurate answer, since the different types of sulphur containing components react at very different rates.
Therefore a classification system has been proposed that groups components with similar reaction behaviour (hydrogenation, desulphurization, etc) and similar reactivity. This reduces the number of rate constants and makes calculations easier. This classification system is given in 15.1 and the proposed reactions are given in 15.1.2.

4.3 Thermodynamics

As can be seen from the heats of reaction in Table 3.1 all reactions are exothermic. The equilibrium lies to the desulpherized products at the temperatures used (~410 ^{0}C), but the rate at which these equilibria are achieved is different. The problem lies in the reactivities as explained in the previous section. Hydrotreating of heavy fractions requires high temperatures and high hydrogen partial pressures compared to hydrotreating of light fractions.

4.3.1 Selection of thermodynamic models

In all units a non-ideal liquid coexists with a non-ideal gas. In the reactor for example, the gas-phase is composed of H_2O, H_2, C1-C5, H_2S, NH_3. This would suggest an ideal-gas, since the molecules are all small molecules.
From literature[12] a gas-phase can be assumed ideal, when the pressure is less then 10 bar. This is certainly not the case here, so the gas-phase is assumed to be non-ideal. The liquid phase is also non-ideal, due to the very different kind of molecules in the streams.
In this case it is therefore better to use an equation of state model like Redlich-Kwong or Peng-Robinson to calculate volumetric and thermal properties of the gas-phase. These calculations are easily done in programs like Matlab or Aspen.
For the liquid phase an activity coefficient model is suitable, like Wilson or Van Laar. From literature [13] it is advised to use the UNIQUAC method, available in Aspen, when many types of components are present and not much parameters from literature.

4.3.2 Operating window and Data validation

A number of thermodynamic data is summarized in Table 15.2. The data is valid for the temperatures and pressures mentioned. They are obtained from information provided by the principles.
To validate the values obtained after calculations with Matlab and Aspen, some literature references are summarized in Table 4.2 and 15.1.

4.3.3 Accuracy

Accurate data on heat capacities and enthalpies are provided by the principals. The only important parameters that will be estimated are the rate constants.

The accuracy needed depends on several factors:

1. The level of design: At this point we are past rough cost estimations. However, no definite decisions involving purchases of equipment or construction are to be made on the results. An advise to continue investigation in this area will be given.
2. The reliability of the design method: Highly accurate rate constants will not add to the reliability of the final composition. Order of magnitude is enough.
3. The sensitivity to the particular property: It was shown before that rate constants are highly temperature dependant.

4.4 Catalysts

Because of the fact that the most difficult molecules desulphurize via the HYD route, a catalyst is needed that promotes hydrogenation as well as desulphurization. Noble metals are much better hydrogenation catalysts than for example metal sulphides. The problem is that these metals can transform into inactive metal sulphides particles in the presence of sulphur-containing molecules like H_2S. The noble metals on the right hand side of the periodic table are less sensitive to sulphur and this characteristic is improved by the use of an acidic support and by alloying.

Noble metals can thus best be used in a second reactor of a two-stage hydrotreater, where the formed H_2S is removed before it enters the reactor and the sulphur content is low enough for the metals to maintain enough activity.

However in this design a conventional metal sulphide catalyst is chosen, because noble metals are very expensive. Moreover, good results can also be obtained with this catalyst.

Nickel is known for its good hydrogenation activity. The combination of Ni with Mo is a classic catalyst in hydrotreating units. This catalyst is also used in the current operation.

It has been mentioned that H_2S strongly inhibits the conversion of DBT and alkyl-benzothiophenes. This is shown in Table 4.2. This also shows that the initial concentration of thiophenes does not affect the conversion.

Table 4.2: Reactivity constants for a NiMo-type catalyst at different initial partial pressures of H_2S [19]

Cat	P_{H2S}(initial)			
NiMo	0	10	35	100
k_{DBT}	2.33	1.06	0.39	0.25
$k_{4.6\text{-}DBT}$	0.2	0.13	0.11	0.08

4.4.1 Nebula

A very promising catalyst used for hydrocracking pre-treatment is the Nebula-20 catalyst, developed and produced by Albemarle. This catalyst has a super high HDS-activity and therefore it can be used for deep desulphurization of middle-Distillate streams, to a sulphur content of around 10ppm. It is used in reactor systems which perform on medium and high pressure (20-100bar). The Nebula-20 catalyst can reach a running time of 2.5 years, 1 year longer than the currently used NiMo catalysts.

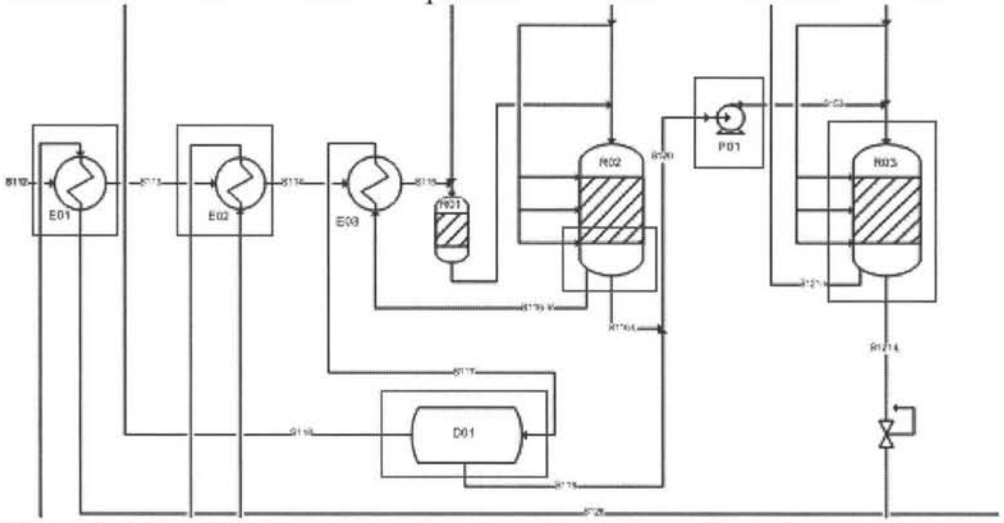
Although the prices of this catalyst, the reaction constants, kinetics and reactive surface are unknown, it still looks like a very interesting catalyst. It can bring the gas oil stream back to a very low sulphur content (>50ppm) without any problem, it can perform under relative high pressures and has a long running time (up to 2.5 years).

5 Process Structure and Description

5.1 Criteria and Selection

In the foregoing chapters a process is chosen to reduce the sulphur content of the GO-finer Distillate stream. It was decided that a new reactor, (RX3), will be used in this design. From here on, the reactor will be called (R03), according to the new process flow scheme shown in figure 5.2.

The hydrogen stream will be fed to the reactors with a semi-counter current configuration. In this paragraph will be explained which units will be used in the new design, in order to fit the design in the current configuration of the GO-finer. Furthermore the way of operating these units is explained. Detailed information on and selection of the units can be found in 8. Detailed explanation of the total design can be found in 5.2 (Process Flow Scheme). A small selection of the process flow scheme is shown in Figure 5.1, in which the new units and equipment are situated.



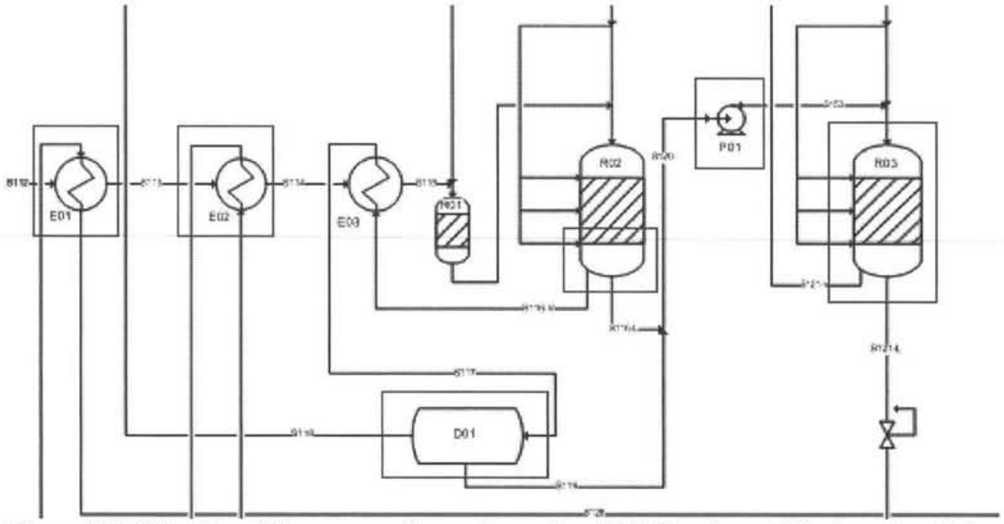


Figure 5.1: Selection of the process flow scheme in which the place of the 'new' units is given.

Reactor 3(R03)

The new reactor is (R03). In this reactor deep desulphurization takes place. The feed for this reactor will be the hydrocarbon stream, mixed with hydrogen. The reactor is filled with catalyst in different beds. Between the beds hydrogen is quenched. Reasons for the quenching are the reduction of the temperature and reducing the partial pressure of H_2S, which inhibit the desulphurization reactions. At the bottom of the reactor, the vapour and the liquid stream are separated with the use of special internals. The vapour will be used as feed for reactor 2 (R02) and the liquid (which contains the end-products) will be further treated and separated.

Changes Reactor 2(R02)

The configuration of reactor 2 (R02) is the same as the one of reactor 3 (R03), although volume, catalyst volume and number of catalyst beds used can vary. The current reactor can not separate a liquid and a vapour stream at the bottom of the reactor. So changes have to be made in order to do this separation, which means the same internals at the bottom of the reactor have to be used as in reactor 3 (R03).

Separator (D01)

The vapour stream from reactor 2 (R02) consist of H_2, H_2S and hydrocarbons. To ensure that the amount of hydrocarbons fed to the HPCS is not too high; a separation of the majority of the hydrocarbons from the H_2 and H_2S is required. This separation is done in separator 1 (D01). The 'old' HPHS will be used as the separator. The liquid stream, the hydrocarbons, is mixed with the hydrocarbon stream from reactor 2 (R02) to reactor 3 (R03). The vapour stream, the H_2, H_2S and the non-separated hydrocarbons, is treated in the HPCS where H_2 and H_2S is separated from the remaining hydrocarbons.

Heat Exchanger 1 (E01) and Heat Exchanger 2 (E02)

Both the liquid and the vapour stream from the LPHS (D02) are at a temperature which is too high for entering the fractionator. Those streams are cooled in heat exchanger 1 and heat exchanger 2 and consequently warming up the feed.

Pump (P01)

Reactor 2 (R02) and reactor 3 (R03) are most likely situated next to each other and gravitational flow is not occurring. Therefore transportation of the liquid stream from (R02) to (R03) is done with the use of a pump (P01). Another function of (P01) is the increase of the pressure of the liquid stream to (R03), because there is a pressure drop in (R02) and the reactions in (R03) still needs to be at a high pressure.

Hydrogen feed

The way H_2 is fed to Reactor 2 (RO2) and Reactor 3 (RO3) is different than the current design. Treat gas from the compressor is mixed with make-up gas. This stream will be split up in two parts. One will be used for quenching in (R02) and for quenching in (R03). The vapour phase of reactor 3 (R03), which still contains a lot of H_2, will be mixed with the feed of the GO-finer. This is done after Heat Exchanger 3 (E03), because the vapour stream is already at high temperature caused by the exothermic reactions occurring in (R03).

5.2 Process Flow Scheme (PFS)

The process flow scheme is the heart of the design. In this paragraph the process flow scheme,(Figure 5.2) will be given together with a process flow description. For better understanding of the process flow descriptions, stream numbers are given with < > and equipment with ( ) signs. Different letters are given for different kind of equipment: R stands for reactor, E for heat exchanger, heater or cooler, D for a drum (separator), C for compressor.

At Heat Exchangers 1 (E01) to 3 (E03) the Cold Feed <S112> (<S113> after (E01), <S114> after (E02) and <S115> after (E03)) is heated with the vapour stream from Reactor 2 <S116V> and with the streams form the LPHS (D02) after reactor 3, <S126L> and <S126V. Heated Feed <S115> will be mixed with Vapour from Reactor 3 <S121V>. The mixed stream goes to Reactor 1 (R01), in which the metals and other contaminations are removed. In this reactor also little desulphurization takes place. After (R01) the stream will be mixed again with Treat Gas to Reactor 2 <S164>. The mixed stream goes to Reactor 2 (R02), in which desulphurization takes place. An amount of <S164> is quenched between the catalyst beds in (R02). This is done in order to control the temperature profile in (R02). At the bottom of (R02), after the last catalyst bed, vapour and liquid are separated with special designed internals. Vapour from Reactor 2 <S116V>, containing H_2, H_2S and hydrocarbons, will be separated in High Pressure Hot Separator 1 (D01). Liquid Reactor 2 <S116L> will be transported to Reactor 3 (R03).

<S116V> is cooled in Heat Exchanger 3 (E03) because the temperature is too high for (D01). The cooled vapour of Reactor 2 <S117> is fed to (D01). In the HPHS, (D01), stream <S118>, which contains mostly hydrogen and other light gases, is separated from the hydrocarbons <S119>.

<S119> is mixed with <S116L>. The mixed stream, <S120>, is pumped to Reactor 3 (R03) by Pump 1 (P01). Liquid feed to Reactor 3 <S153> is mixed with treat gas to Reactor 3 <S150>. The mixed stream will enter (R03). In this reactor deep desulphurization takes place. An amount of <S150> is quenched between the catalyst beds in order to control the temperature profile in (R03). At the bottom of (R03), after the last catalyst bed, vapour and liquid are separated with special designed internals. Vapour from Reactor 3 <S121V> will be mixed with the feed of reactor 1 <S115>. The liquid from Reactor 3 <S121L> is send to the LPHS or (D02). A pressure relief valve is used to lower the pressure.

The vapour and liquid streams of (D02), <S116L> and <S116V> are used to heat the fresh feed to the reactor system. Heat exchangers 1 and 2, (E01) and (E02) are used for this purpose.

The HPCS feed, <S118>, is mixed with steam, <S124>. Mixing with steam is required to lower the partial pressure of the existing hydrocarbons in <S118> and to make the dissolving of nitrogen salts and H_2S in the HPCS (D07) more effective. The mixed stream, <S129>, is cooled in a series of Heat Exchangers, shown as one exchanger (E10). The cooled stream, <S130> is fed to the HPCS (D07).

In the HPCS three phases are present, a water phase, a liquid hydrocarbon and a vapour phase. Sour gases, like H_2S and NH_3 will partially dissolve in the water phase to form sour water <S132>. The sour water will be transported to an off-site treating unit. The liquid hydrocarbon stream, <S133> contains mostly naphtha and will be transported to the fractionator unit. The vapour phase of the HPCS, leaving over the top as <S131>, contains reasonable quantities of sour gases and is therefore treated in the MEA scrubber (D08).

In the MEA Scrubber (D08), <S131> will be treated with a lean MEA stream. The remaining H_2S and NH_3 will dissolve in the MEA. The rich MEA stream will go to a MEA recycle unit. MEA Out <S134>, which mainly consists of H_2, will be split in a Purge <S152> and the compressor feed <S135>. A purge of <S134> is added before the compressor because of the constraint on the compressor.

<S135> is compressed in the Compressor (C01). Compressed treat gas <S136> will be mixed with Make-Up Gas 1 <S162> to increase the partial pressure of H_2. Total treat gas feed <S163> will be fed back to the reactors and will be split up in <S164> and <S150>.

The outlet streams of the LPHS, <S126L> and <S126V>, are cooled with cold fresh feed in heat exchangers (E01) and (E02) and send to the fractionator. The liquid cooled outlet, <S154>, is mixed with steam <S157>, which will reduce the partial pressure of the hydrocarbons and therefore lower the operating temperature of the Fractionator (D03). The cooled vapour outlet, <S128>, is mixed with the top stream, <S144>, of the side stripper (D05) and sent to the fractionator (D03), <S137>. <S137> enters the fractionator (D03) at stage 20.

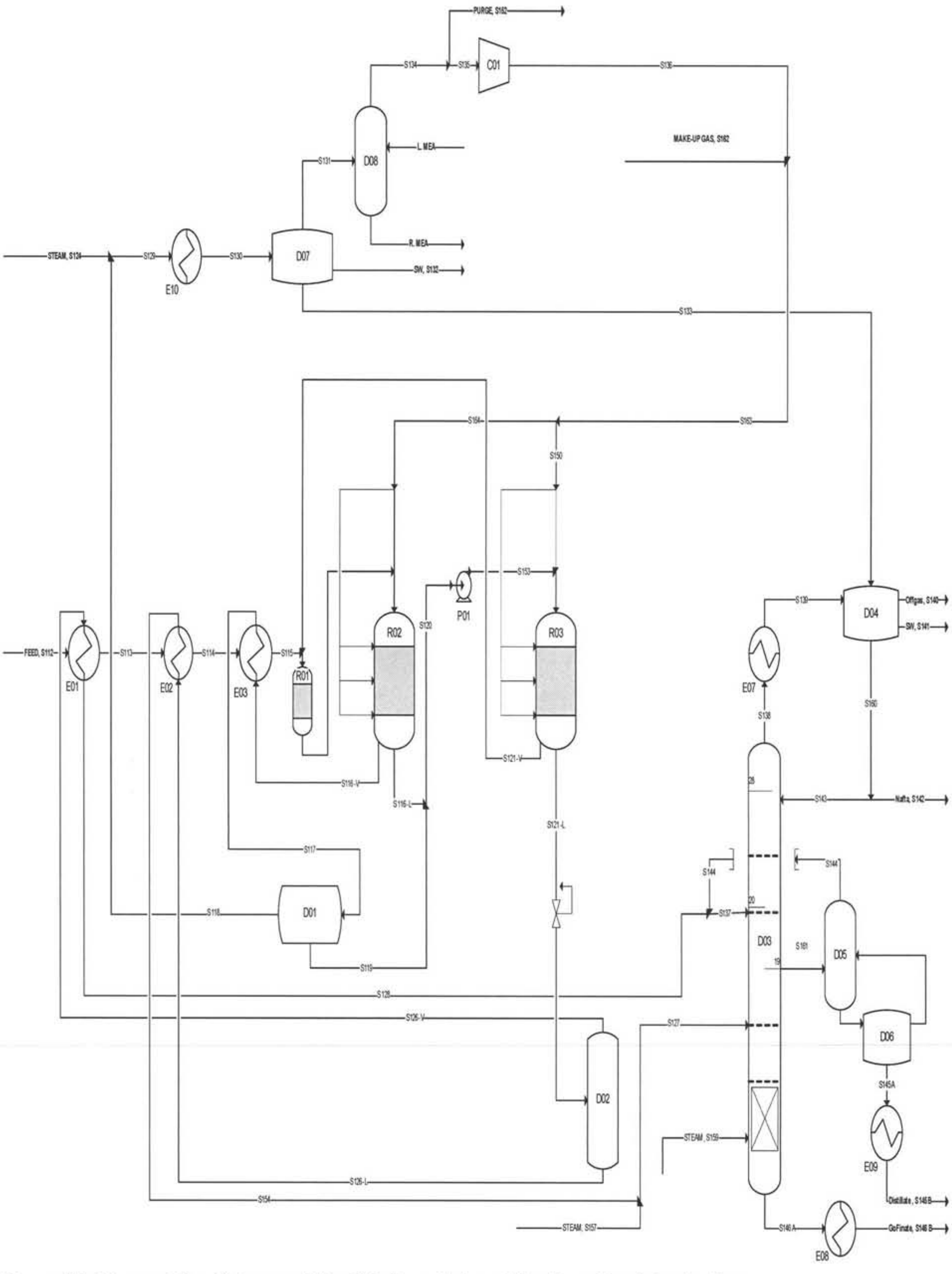
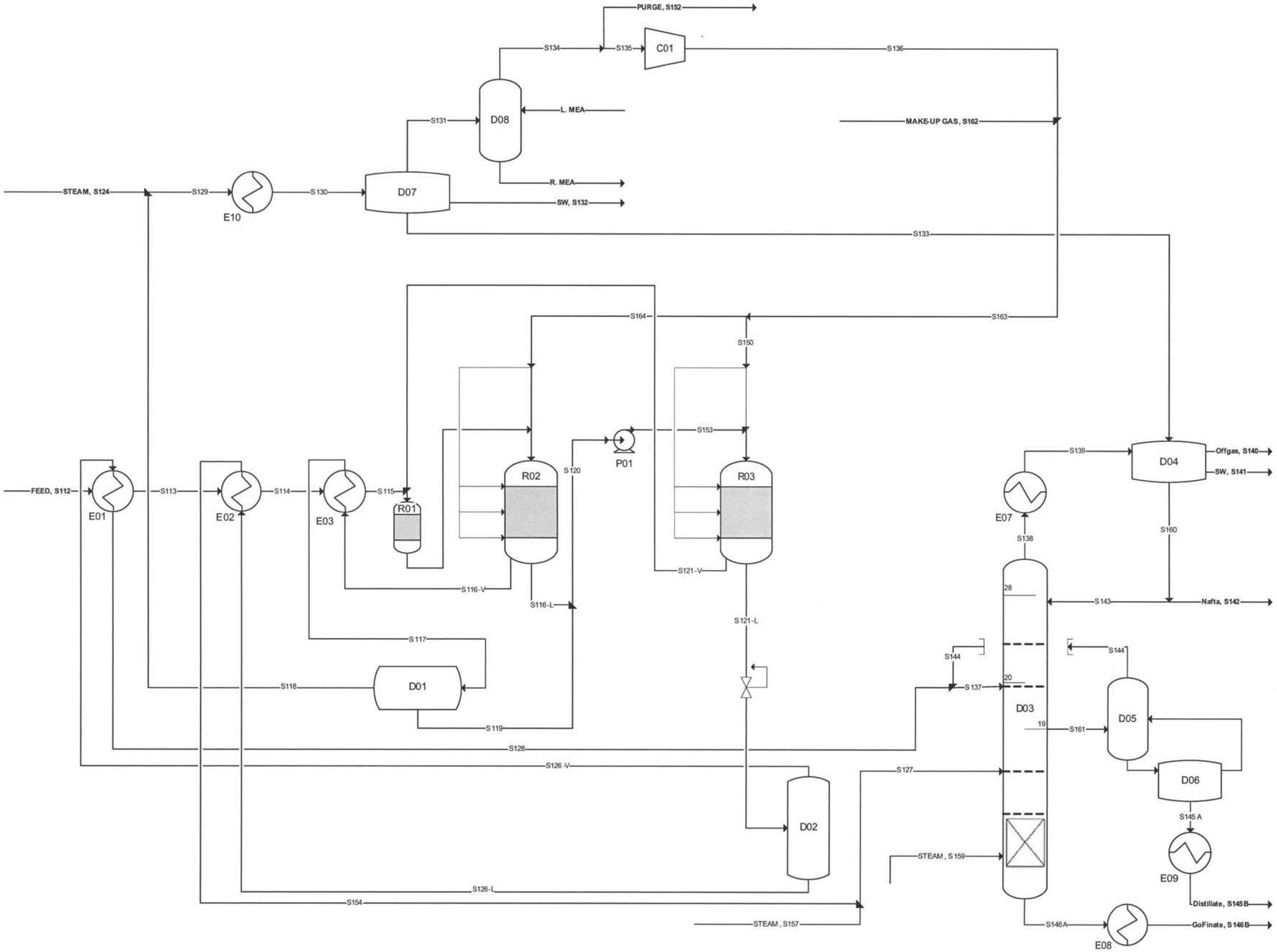


Figure 5.2: Process Flow Scheme of the GO-finer designed for deep desulphurization.


PURGE, S152
S134
S135
C01
S136
D08
L. MEA
S131
MAKE-UP GAS, S162
STEAM, S124
S129
E10
S130
D07
R. MEA
SW, S132
S133
S164
S163
S150
S153
P01
R02
R03
R01
S120
FEED, S112
E01
S113
E02
S114
E03
S115
S116-V
S116-L
S121-V
S121-L
S117
D01
S118
S119
S128
S126-V
D02
S126-L
S154
STEAM, S157
S127
STEAM, S159
S139
D04
Offgas, S140
SW, S141
E07
S138
S160
28
S143
Nafta, S142
S144
S144
20
S137
D03
19
S161
D05
D06
S145 A
E09
Distillate, S145B
S146A
E08
GoFinate, S146B

At the bottom of (D03) steam <S159> is injected. This is done to strip the bottom product and to reach the GO-Finate flashpoint specification.

The Fractionator (D03) separates the products of the GO-Finer product. The bottom product is the GO-Finate <S146A>. The 'middle' product is the Distillate. It leaves (D03) in Distillate Frac Out <S161>. Via drums (D05) and (D06) a certain amount is refluxed back to (D03). The reflux, Reflux Frac Distillate <S144>, is mixed with <S128>. Go-Finer Distillate <S145A> is the part that is not refluxed back.

The top product of (D03), Frac Top Out <S138> is condensed in Heat Exchanger 7 (E07). Cooled Frac Top Out <S139> is fed to Drum 4 (D04). Also Hydrocarbons HPCS Out <S133> are fed to (D04). In this drum, the light fractions are separated in offgas <S140>, sour water <S141> and Hydrocarbon Liquid (D04) <S160>. <S140> is sent back to the Flexicoker. <S141> is transported to an off-plant treatment unit. <S160> is split in two fractions. Frac Top Reflux <S143> and naphtha <S142>. <S143> is the reflux of the top products and fed to (D03). <S142> leaves the GO-Finer as product.

5.3 Process Stream Summary

The complete process stream summary can be found in 15.2.

5.4 Utilities

For a general overview of the utilities used in the new design, a Utility Summary is made and can be found in Table 5.1. Utilities in this table are required for the new units and equipment. Utilities used in current equipment, is assumed not to change in the new design.

Table 5.1: Summary of Utilities (only required utilities for the new units are determined; other utilities are assumed to be constant or not changing in the new design)

SUMMARY OF UTILITIES											
EQUIPMENT		UTILITIES									
		Heating					Cooling		Power		REMARKS
Nr.	Name	Load	Consumption (t/h)				Load	Consumption (t/h)	Actual	Consumption (t/h, kWh/h)	
			Steam					Cooling	Load	Electr.	
		kW	STM-1	STM-3	STM-9	STM-40	kW	Water	kW	kWh/h	
P01	Liquid Pump								152	152	Pumping of Liquid between (R02) and (R03)
C01	Compressor								-	-	Compression of treat-gas from MEA
TOTAL									152	**152**	

Remark: The compressor is not taken into account, because the power used in the current situation (701kW) is higher than the one in the new situation (680kW). No extra power is required and therefore not taken into account in this utility sheet.

5.5 Process Yields

Process Yields represents the consumption of feed, products and utilities per amount of product produced (Distillate in this case). In Table 5.2 the process yields of process streams is given and in Table 5.3 the process yields of utilities is given.

Table 5.2: Process Yields summary of Process Streams

Process Streams							
Name	Ref. Stream	kg/s		t/h		t/t Distillate	
		IN	OUT	IN	OUT	IN	OUT
Cold Feed	<S112>	38.9		140.0		1.88	
Make-Up Gas	<S162>	3.1		11.0		0.15	
Steam	<S124>	5.6		20.0		0.27	
	<S157>	0.3		1.0		0.01	
	<S159>	1.9		7.0		0.09	
GO-Finer Distillate	<S145B>		20.7		74.5		**1.00**
GO-Finate	<S146B>		16.7		60.0		0.81
GO-Finer Naphta	<S142>		2.1		7.4		0.10
Off-Gas	<S140>		0.8		3.0		0.04
Sour Water	<S141>		2.2		8.0		0.11
	<S132>		5.8		20.8		0.36
Purge	<S152>		0		0		0
Total		49.8	48.3	179.0	173.7	2.40	2.42

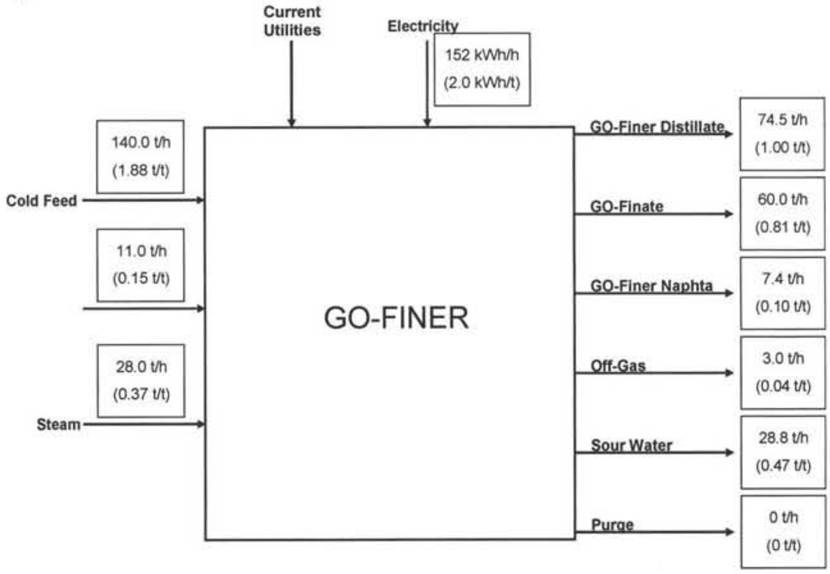
Differences between the streams IN and OUT are caused by the fact that the MEA streams are not taken into account in the process yield of the process streams.

Table 5.3: Process Yields summary of Utilities

Utilities							
Name	Ref. Stream	kg/s	kW	t/h	kWh/h	t/t Distillate	kWh/t Distillate
Electricity	-		152		152		2.0

A schematic overview of the process can be made with the use of the tables above. This schematic overview can be found in Figure 5.3.

Figure 5.3: Schematic Overview of Process Streams and Utilities



6 Process control

It was agreed with the principal to only discuss the process control for new equipment. The existing process control system is left untouched; it probably needs new set points but the determination of set points for controllers is not the scope of this report.
The newly introduced equipment consists of one reactor, two heat exchangers and one pump. Because the configuration of the reactor section has changed significantly the whole system will be discussed. Controlling the temperature is the main objective in the reaction section. The pump is placed between the current and new reactor but does not need additional control.

6.1 Heat exchangers control

There are several heat exchangers all with a different approach to controlling the temperature. If two process streams are involved the following approach works best:

- Heat the cold process stream to the specific temperature using a bypass with a temperature controlled valve to prevent too high temperatures.
- The hot stream should be further cooled by an additional installed cooler.
- A temperature controller should adjust the flow stream of the cooling water or a bypass for the process stream can be used with a temperature controlled valve. If the flow rate of the cooling water is not easily adjustable the first option should not be chosen. If fouling is a main concern the last option should not be chosen; the bypass reduces the flow through the cooler and therefore the flow rate.

Because heat exchangers 1 to 3, (E01) to (E03), are used in a slightly different way then in the current process a control structure for these heat exchangers is suggested. Because all three are used to heat the cold feed to the reactor system the control structure is the same for all three. For this reason only one will be discussed.
For the operation of the GO-finer it is important that the streams to the fractionator and to the HPCS have a certain temperature. Therefore it is suggested that the temperature of these streams are controlled. The feed of the reactor goes through all three heat exchangers and therefore the temperature of this stream is more difficult to control. In Figure 6.1 the control structure is given for (E03) and as mentioned the same structure should be used for (E01) and (E02). The control valve should be placed in the feed to the reactor system and the temperature measurement should be done in stream <S154> and <S128>.

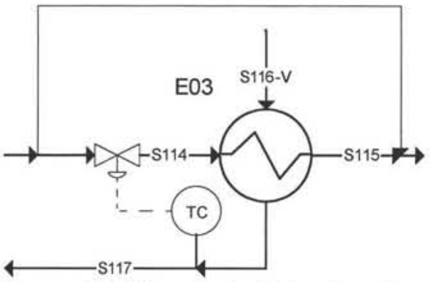


Figure 6.1: The control structure for heat exchanger (E03)

6.2 Reaction section control

The amount of hydrogen entering the system of (R01) and (R02) depends on the amount leaving (R03). The quench needed to keep the temperature profile within the given restrictions can be adjusted by valves controlled by temperature controllers. The temperature in the reactors needs to be measured to accomplish this. The hot process stream leaving (R02) and entering (R03) is mixed in the top of (R03) with cold hydrogen. The quench for (R02) and (R03) and the hydrogen entering (R03) should be controlled since all streams are supplied by one pipe. The absolute amount of hydrogen entering (R03) can be controlled by a flow controlled valve. Another option is a ratio controller, but as long as the feed to the reactor system is constant in amount, a flow controller works well enough. In Figure 6.2 a detail of the process flow sheet is presented with the control structure of the reactor system.

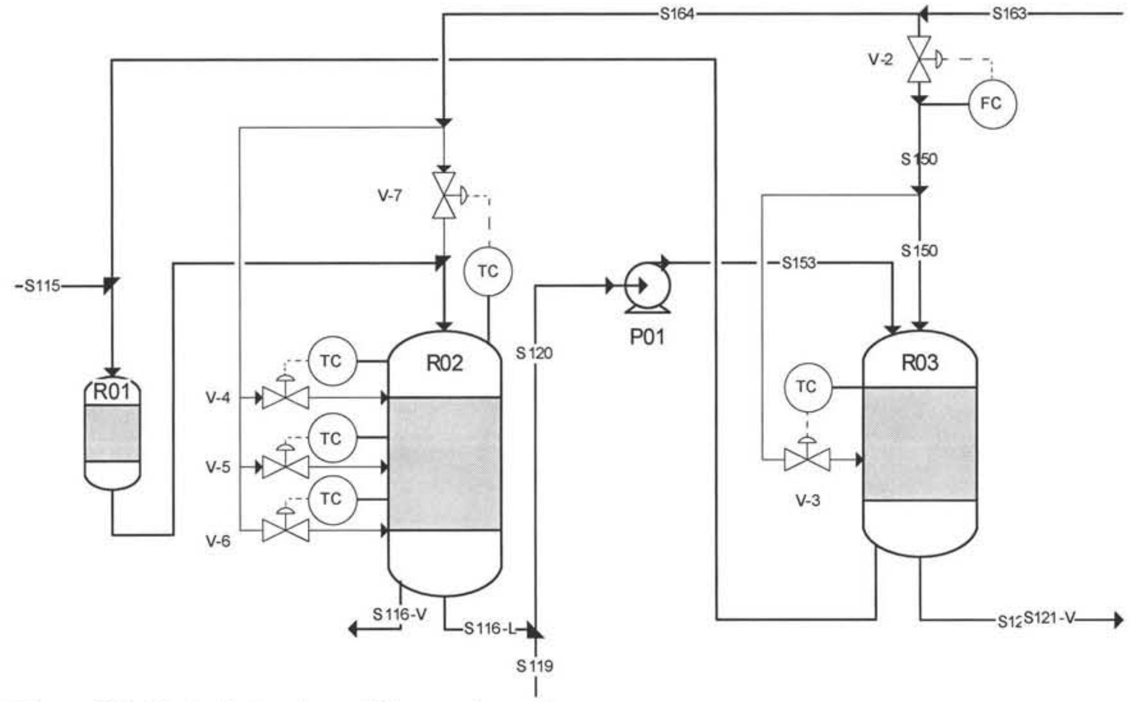


Figure 6.2: Control structure of the reactor system

7 Mass and heat balances

7.1 Equipment mass and heat summary

The equipment mass and heat summary summarises the in- and outlet streams per equipment. The equipment mentioned can be found in the PFS as represented in 5.2.

Table 7.1: Equipment mass and heat summary

IN					Equipment	OUT				
Plant		Equipment				Equipment			Plant	
Mass Kg/hr	Heat Kw	Mass Kg/hr	Heat Kw	Stream Nr.	Identification	Stream Nr.	Mass Kg/hr	Heat Kw	Mass Kg/hr	Heat Kw
		140.000	-40.425	<S112>	**E01**	<S113>	140.000	-36.845		
		37.503	-4.293	<S126-V>		<S128>	37.503	-6.336		
		177.503	-44.719		Total		177.503	-43.182		
		140.000	-36.845	<S113>	**E02**	<S114>	140.000	-34.802		
		93.357	-18.367	<S126-L>		<S154>	93.357	-21.947		
		233.357	-55.212		Total		233.357	-56.749		
		140.000	-34.802	<S114>	**E03**	<S115>	140.000	-30.449		
		44.672	-4.155	<S116-V>		<S117>	44.672	-8.508		
		184.672	-38.958		Total		184.672	-38.958		
		140.000	-30.449	<S115>	**R01/R02**	<S116-V>	44.672	-4.155		
		28.365	-4.114	<S121-V>		<S116-L>	129.348	-23.693		
		5.684	-2.892	<S164>						
		174.049	-37.456		Total		174.020	-27.848		
		145.831	-27.565	<S120>	**P01**	<S153>	145.832	-27.413		
		145.832	-27.413	<S153>	**R03**	<S121-V>	28.365	-4.114		
		13.262	-6.748	<S150>		<S121-L>	130.860	-25.274		
		159.094	-34.161		Total		159.225	-29.388		
		44.672	-8.508	<S117>	**D01**	<S118>	28.189	-5.596		
						<S119>	16.483	-3.872		
								959		**959**
		44.672	-8.508		Total		44.672	-8.508		
		130.860	-25.274	<S121-L>	**D02**	<S126-V>	37.503	-4.293		
						<S126-L>	93.357	-18.367		
	2.613		**2.613**							
		130.860	-22.660		Total		130.860	-22.660		
		94.357	-25.509	<S127>	**D03**	<S138>	70.347	-44.174		
		39.362	-6.547	<S137>		<S146A>	60.000	-7.770		
		66.049	-26.831	<S143>		<S161>	76.421	-16.921		
		7.000	-25.121	<S159>						
	15.143		**15.143**							
		206.768	-68.865		Total		206.768	-68.865		
		70.347	-44.174	<S138>	**E07**	<S139>	70.347	-60.835		
								16.661		**16.661**
		70.347	-44.174		Total		70.347	-44.174		
		14.047	-5.590	<S133>	**D04**	<S140>	2.976	-1.720		
		70.347	-60.835	<S139>		<S141>	8.031	-35.027		
						<S160>	73.388	-29.813		
								134		**134**
		84.394	-66.425		Total		84.394	-66.425		
		76.421	-16.921	<S161>	**D05**	<S144>	1.859	-210		
						<S145>	74.562	-13.874		
	2.838		**2.838**							
		76.421	-14.083		Total		76.421	-14.084		
		48.189	-93.272	<S129>	**E10**	<S130>	48.189	-102.359		
								9.087		**10.901**
		48.189	-93.272		Total		48.189	-93.272		
		48.189	-102.359	<S130>	**D07**	<S131>	13.320	-5.556		
						<S132>	20.821	-91.211		
						<S133>	14.047	-5.590		
	3		**3**							
		48.189	-102.357		Total		48.189	-102.357		
		13.320	-5.556	<S131>	**D08**	<S134>	12.352	-23.669		
		85.826	-246.142	L.MEA		R.MEA	86.794	-228.336		
								307		**307**
		99.146	-251.698		Total		99.146	-251.698		
		12.353	-23.669	<S135>	**C01**	<S136>	7.946	-3.820		
						WATER	4.407	-19.169		
	680		**680**							
		12.353	-22.989		Total		12.353	-22.989		

It was found that, except for the reactors, all equipment complies with the laws of mass and energy conservation. The reactors were simulated (as mentioned in 8.1) in a fashion that is not normal practice in Aspen. In and outlet streams thus differ. For a more detailed explanation see 8.1. (E01) and (E02) do not comply with the law of energy conservation within their own system. However, as heat integration is applied, within the heat exchanger system the law of energy consumption is complied with.

7.2 Component mass and heat summary

The component mass and heat summary shows that the equipment summary is correct. In the equipment summary we also have a mass surplus of 760 kg/h. This amount can also be found in Table 7.2. This is also caused by the Aspen simulation.

Table 7.2: Component mass and heat summary

	IN		OUT		IN-OUT	
	Kg/h	Kmol/h	Kg/h	Kmol/h	Kg/h	Kmol/h
H2	6050,00	3001,17	534,60	265,19	5515,40	2735,98
H20	74003,00	4107,79	74110,30	4113,68	-107,30	-5,89
MEA	40000,00	654,84	40000,00	654,84	0,00	0,00
NH3	125,00	7,34	867,85	50,96	-742,85	-43,62
C3	440,00	9,98	338,39	7,67	101,61	2,30
C1	1925,00	119,99	542,50	33,82	1382,50	86,18
H2S	358,00	10,50	5057,99	148,41	-4699,99	-137,90
C2	660,00	21,95	110,09	3,66	549,91	18,29
IC4	110,00	1,89	258,80	4,45	-148,80	-2,56
NC4	198,00	3,41	199,71	3,44	-1,71	-0,03
NC5	77,00	1,07	766,25	10,62	-689,25	-9,55
CYCLOPEN	0,00	0,00	699,97	9,98	-699,97	-9,98
ISOHEX	0,00	0,00	573,22	6,65	-573,22	-6,65
NC6	880,00	10,21	870,11	10,10	9,89	0,11
C02	0,00	0,00	0,00	0,00	0,00	0,00
PC185C	796,23	5,69	795,70	5,68	0,53	0,00
PC198C	1176,03	7,97	1174,90	7,96	1,13	0,01
PC212C	1374,14	8,79	1372,17	8,77	1,96	0,01
PC226C	1667,37	10,06	1663,93	10,04	3,44	0,02
PC240C	2251,67	12,83	2244,83	12,79	6,85	0,04
PC254C	5493,54	29,58	5470,26	29,46	23,28	0,13
PC267C	5066,04	25,91	5037,59	25,76	28,45	0,15
PC281C	5301,36	25,70	5262,22	25,51	39,14	0,19
PC295C	5259,72	24,20	5209,87	23,97	49,85	0,23
PC309C	5196,81	22,70	5134,96	22,43	61,85	0,27
PC323C	5463,25	22,68	5383,52	22,34	79,74	0,33
PC337C	6653,22	26,26	6536,89	25,80	116,33	0,46
PC350C	6221,64	23,44	6095,69	22,96	125,95	0,47
PC364C	4258,29	15,29	4160,53	14,94	97,75	0,35
PC378C	3496,12	11,97	3407,98	11,67	88,15	0,30
PC392C	3580,07	11,70	3485,73	11,39	94,34	0,31
PC406C	4824,73	15,04	4702,58	14,66	122,15	0,38
PC420C	11104,62	33,16	10882,83	32,50	221,80	0,66
PC439C	10642,04	29,96	10899,60	30,68	-257,56	-0,73
PC470C	11362,94	29,24	12260,18	31,55	-897,24	-2,31
PC495C	13031,25	31,17	13040,28	31,19	-9,04	-0,02
PC523C	9911,95	22,01	9912,15	22,01	-0,19	0,00
PC549C	7631,74	15,85	7631,29	15,85	0,45	0,00
PC578C	2738,43	5,30	2738,30	5,30	0,14	0,00
PC607C	2082,97	3,78	2082,91	3,78	0,06	0,00
PC635C	1735,30	2,96	1735,27	2,96	0,03	0,00
PC664C	1678,52	2,70	1678,51	2,70	0,01	0,00
	Total IN	Total IN	Total OUT	Total OUT	Difference	
	264826,00	8426,07	264930,42	5798,14	-104,42	2627,93

8 Process and equipment design

8.1 Process simulation

The process has been simulated using Matlab® for the reaction section and Aspen® for the overall process. This simulation is done for the following reasons:

1. Computing mass and energy balances and utility usage.
2. Modeling the treat-gas recycle, to determine if the flow through the compressor is not exceeding its capacity.
3. Modeling the fractionator, to obtain pseudo-component distribution for the products.
4. Obtaining values for rate constants based on current equipment and computing new reactor volumes

Simulating this process was not straightforward. It should be clear after reading 4.1 that the reactions occurring in the reactor are difficult to model or predict, since there are many components that are all reacting with hydrogen and competing for the catalyst. Secondly, Aspen ® cannot simulate a reactor when pseudo-components are used.

Therefore the reactor has been designed in Matlab® using the reactions and equations previously described in 4.1. The hydrogen consumption obtained was used in Aspen to model the complete process.

8.1.1 Aspen® simulation of the process

The process that is simulated is simplified compared to a real-life process, like the current Go-Finer. Heat exchangers have been lumped into one unit and some equipment, like valves, storage drums and process control units, has been left out. The process flow-sheet shown in 5.2 is used as a basis for the simulation. In Aspen® pseudo-components have been generated using True Boiling Point (TBP) data available for the feed. The input data used and specifications to be met are summarized in Table 15.3.

The compressor capacity is: maximal 1597 m^3/hr, minimum 815 m^3/hr. This constraint is managed by a purge before the compressor.

Furthermore it is ensured that the hydrogen recycle has less than 0.1% H_2S. Temperatures and pressures for reactors, some flash drums and fractionator, used are copied from the current process.

- ***Reactor configuration***

In the BOD it was decided to use a reactor that has separated exits for the gas and vapour streams. In doing simulations it became clear that the vapour stream leaving (R02), <S116-V> needs to be cleared of light hydrocarbons. Otherwise they would be sent to the cold separator (D07) increasing this stream beyond the capacity. The flash-drum added is the same HPHS used currently (D01). It is operated at a slightly lower temperature, to ensure that enough hydrocarbons are condensed. The stream needs to be cooled before it is sent to (D01). This is done by exchanging heat with the cold feed <S112>.

The liquid stream leaving (R03) contains a neglectable amount of light gasses. Therefore treating this stream in a HPHS is not necessary anymore. The stream can be sent to the LPHS (D02) currently used.

Because of the fact that this stream is now heavier, the D02 overhead would be very small if it were operated at the same temperature as it is currently (344^0C) done. (D02) is therefore operated at a higher temperature (400^0C) and lower pressure (3 bar).

This has also consequences for the heat integration. The reactor effluent is 400^{0}C and needs to be cooled to approximately 340^{0}C. This is currently done by heat integration with the LPHS overhead, which used to be 344^{0}C. The temperature of the overhead is now 400^{0}C, which makes heat integration now clearly impossible and also unnecessary.
The reactor effluent stream is now sent directly to (D02) . The vapour and liquid effluents of (D02) are both used to heat the cold-feed <S112> using heat exchangers. These have a different heat-exchanger area, so the current heat-exchangers cannot be used.

- ***Treat-gas make-up and recycle***

The treat-gas make-up is determined by a design specification: The make-up will be such that the treat-gas to be mixed with the feed and for quench <S163> always contains 11000 kg/hr of hydrogen.
This is because this stream is split and sent to (R02) and (R03) as quench gas and 'reacting' gas. The reason for choosing this stream for quench, is because it already has the right temperature after the compressor. The gas-effluent from (R03) is now mixed with the feed to (R02), to pre-heat the feed.

- ***Product specifications***

It was difficult to get the specified standard API gravity's for the product streams. This is caused by the fact that the treat-gas used in simulation differs from the treat-gas used in the real process. There are less light gasses in the process, because some gasses have been left out for simplicity.
Secondly it was also difficult to get the right specifications for the reactor effluent. Aspen cannot simulate a reactor when pseudo-components are used. The reactor has been simulated by a series of separators, which use split-fractions to designate components to different streams.
Products formed are just added to the streams, and reactants are removed from the streams. This also has consequences for the product compositions, because the streams differ from real-life.
Furthermore the material 'entering' the reactor and 'leaving' the reactor, representing reactants formed and reacted, are not the same. This would suggest that mass is disappearing, which is of course impossible. This also causes the imbalances in the mass and heat balances in 7.1.

- ***MEA-unit***

The MEA-unit has not been simulated as an extractor, but also as a separator. For some reason Aspen could also not calculate an extraction and needed an un-feasible amount of MEA to extract about the same amount of hydrogen sulphide as is currently used. It was not within the scope of the assignment to design the MEA unit, so detailed simulation of this unit is not done.

- ***Fractionator***

The fractionator has not been changed compared to the current operation concerning the equipment, except for the bottom. Aspen could not model the fractionator without either a condenser or a reboiler. Therefore a reboiler is added, which in fact is the external reboiler for the GO-Finate used currently. Heat duty's and refluxes are different and also a pressure drop of 0.1 bar per stage is assumed.

8.1.1.1 Sensitivity analysis

- *The effect of the feed (146 and 152) position on density*

It has been found that the density of the Distillate and the GoF8 does not change with the variation of the feed position.

- *The effect of the position of stream 154*

The densities are compared when the stream is fed directly to the column and when the feed is entered as reflux. As can be seen from Table 8.1 the density does not change mentionable.

Table 8.1: Densities of Distillate and GO-Finate

	154 in reflux	154 in column
Distillate	662	662
GO-Finate	577	576

- *The effect of the number of theoretical trays*

It has been found in simulation that increasing the number of trays increases the GoF8 density. It is chosen however to operate the fractionator with the same amount of trays as currently used, because otherwise it would mean extra investment costs.

- *The effect of the reflux ratio on the heat duty and density*

Increasing the reflux increases the heat duty of the reboiler, but also destabilizes the vapour-liquid equilibrium on a tray. There is therefore a maximum to the reflux ratio. This is around 0.9 (90% of <S190> is sent back).
There is also a maximum to the amount of liquid that can be drawn for Distillate, for the same reason as mentioned before. This maximum is 26.5% of the total feed.

8.1.1.2 Overall conclusion

The new design needs some new equipment: the reactor and the internals of the current reactor and heat-exchangers. The treat-gas recycle is within the constraints given.
Further investigation needs to be done concerning the right vapour compositions of the reactor effluents, obtaining the right densities of the product streams.

8.1.2 Matlab® simulation of the reactor

When designing a reactor several issues are important. Besides the valid phases within the reactor, the internals (like the type and distribution of a catalyst) and distribution of the valid phases, the volume of the reactor is important. The volume of the reactor can be calculated based on mass balances, which need kinetic parameters for all involved reactions. Since properties and kinetic parameters of most of the components involved were not known estimations needed to be made. Matlab ® was used for this purpose.
The project principal provided component distributions for the feed, Distillate and GO-Finate. This gave a good indication of the conversions of the different components. Together with the mentioned reaction scheme presented in 15.1.2, an optimization procedure was started to calculate the values of all kinetic parameters. As long as the operating conditions do not differ from the current situation, the kinetic parameter values, which are a strong function of temperature, can be considered constant.
Matlab ® provides several optimization functions, but the severe number of reactions (138) and components (132) resulted in simulation problems. A good initial estimation for the kinetic parameters is a necessity in such cases and even then patience is required. After evaluating the provided functions and the error still present, it was decided to optimize by hand. This meant changing one kinetic parameter until the involved reactant reached the desired value; the simulated reactor outlet should match the provided component distribution.

Especially the sulfur and nitrogen containing components needed to be accurately simulated because the content of these components are of particular interest.
Once the values of the kinetic parameters resulted in a simulated components distribution that did not differ more then 2% from the provided component distribution for the components of interest, the optimization was stopped. The kinetic parameters where then used to calculate the volume of the new reactor. The specification for the sulphur content was the determining factor. Because only the Distillate should reach 50 ppm S, the overall sulphur content can be 225 ppm S. Based on the provided component distribution and the assumption that the split fraction of sulphur containing components over GO-Finate and Distillate would remain the same, the overall sulphur content can be 225 ppm S. The Distillate then contains 47.5 ppm S and the GO-Finate 480 ppm S.

8.1.2.1 Assumptions for the Matlab ® simulation

The provided component distribution is used to calculate the kinetic parameters and volume of the new reactor. It is important to notice that the sulphur content of the feed was higher then mentioned in other provided information sources. Based on the hydrogen content of the feed and the product given in the component distribution, the hydrogen consumption is higher then reported in the heat and material balances. This will result in higher hydrogen consumptions for both the kinetic parameters calculation and the volume of the new reactor. If the component distribution gives either too low hydrogen content in the feed or too high hydrogen content in the products, the hydrogen consumption is overestimated. Because hydrogen costs are high and an important economic parameter, it is important to validate the component distribution.
It was assumed during the simulation that the operating conditions in the reactor, i.e. temperature and pressure, stayed within the range of the current operation. The components present in the provided component distribution and H_2, H_2S and NH_3 were explicitly taken into account, the lighter components (gases) were lumped as one component with an average molecular weight. Only H_2S was used as inhibitor and because the current operation has a vapour fraction of 0.5, it was assumed that only half of the H_2S remained in the liquid when calculating the inhibition effect. In this way the inhibition effect of H_2S is over estimated but inhibition of other components was neglected. For the estimation of the inhibition parameters of H_2S the literature [20] was used.
For the reaction kinetics molar flows are used where normally concentrations in the liquid or even at the catalyst surface are more common. Because mass transfer coefficients and vapor fraction of all the components were not known, taken this all into account would only add more unknowns to estimate. It was therefore chosen to lump all the unknowns in one 'kinetic' parameter per reaction. In 15.7.2 the used model is described briefly, it is based on the ideal plug flow reactor.
When calculating the new configuration of reactors it was assumed that only H_2, H_2S, NH_3 and the light gases ($C_1 - C_4$) would leave the reactor as vapour. The vapour is send to a HPHS or (R02), depending on the reactor it came from. It was chosen to work with a semi-counter current mode of operation, which means that the vapour from (R03) goes to (R02) (actually R01 and (R02) and the vapour from (R02) goes to the hydrogen recycle (starting with a HPHS). The liquid (feed) goes through (R01), (R02) and (R03) in the mentioned order.
Although more components will leave (R02) as vapour, the amount that will enter (R03) is over estimated, which will result in a conservative estimation for the reactor volume of (R03). This can be concluded when one considers that the lumped kinetic parameter used contains the volumetric flow rate, see 15.7.2.

Of course, the reaction scheme, mentioned in chapter 4, is an assumption it self. It is likely that more reactions can and will take place. The main reactions are taken into account and the overall provided component distribution could be simulated well with some exceptions.

The last assumption was the disregarded guard reactor. The guard reactor was expected to remove heavy metals without performing desulphurization or denitrofication. The heavy metals were therefore also neglected in the simulation of the reaction system.

8.1.2.2 Results of the Matlab® simulation

In 15.7.5 the Matlab ® scripts used can be found.

The distribution of saturates was not perfectly simulated but overall the amount of saturates did match the overall amount of saturates. All the sulphur and nitrogen containing components did match with less then 2% error.

In 15.7.4 the kinetic parameters of the simulated reactions and the mass streams of the components can be found, the main results of the Matlab ® simulation will be given here. The volume of the catalyst bed of the new reactor (R03) is 64 m^3. This is based on minimized hydrogen consumption (see 8.1.2.3) of 7.88 t/h, a hydrogen inlet for (R03) of 7.85 t/h a hydrogen quench of 3.1 t/h and 1.25 t/h for (R02) and (R03) respectively and a hydrogen outlet for (R02) of 4.32 t/h. In Table 8.2 the sulphur and nitrogen content after (R02) and (R03) are given.

It is important to notice that the Distillate is just meeting the specifications and that the influence of the hydrogen entering the reactors is greatly influencing the required reactor volume. (see 8.1.2.3). It is not investigated if the catalyst volume will be enough to desulphurize the feed to the specifications at the end of run. It could therefore be prudent to install a somewhat larger new reactor.

Another important aspect of the Matlab ® simulation is that the hydrogen addition is higher then simulated with Aspen ®. The recycle of hydrogen however is more or less then same. Simulating only parts of a process in different simulation software packages with different approaches will always result in small differences. Matlab ® is based on the component distribution provided by Exxon Mobil and on real components. Aspen ® however is based on pseudo components.

Table 8.2: Sulphur and Nitrogen content of reactor outlets

Reactor outlet	S-content [t/h]	S-content [wt%]	N-content [t/h]	N-content [wt%]
(R02)	1.1487	0.9122	0.1761	0.1398
(R03)	0.0273	0.0224	0.0003	0.0003

8.1.2.3 Sensitivity analysis

A sensitivity analysis was performed to determine the influence of the added hydrogen and the required reactor volume to reach the sulphur specification. As is previously mentioned, the recycle of treat gas is limited. According to the provided heat and material balances the current treat gas recycle contains 6.1 t/h of hydrogen when passing the compressor. Therefore the maximum hydrogen content of the gas-outlet from (R02) is taken as 6.3 t/h to make sure to be within the compressor constrains.

The main conclusions are that higher hydrogen content in the reactor system leads to a smaller (R03) and the hydrogen consumption decreases slightly. The optimum with respect to the hydrogen consumption is 7.88 t/h to (R03) and a reactor volume of 64 m^3 for (R03).

In Figure 8.1 and Table 8.3 these conclusions are also shown.

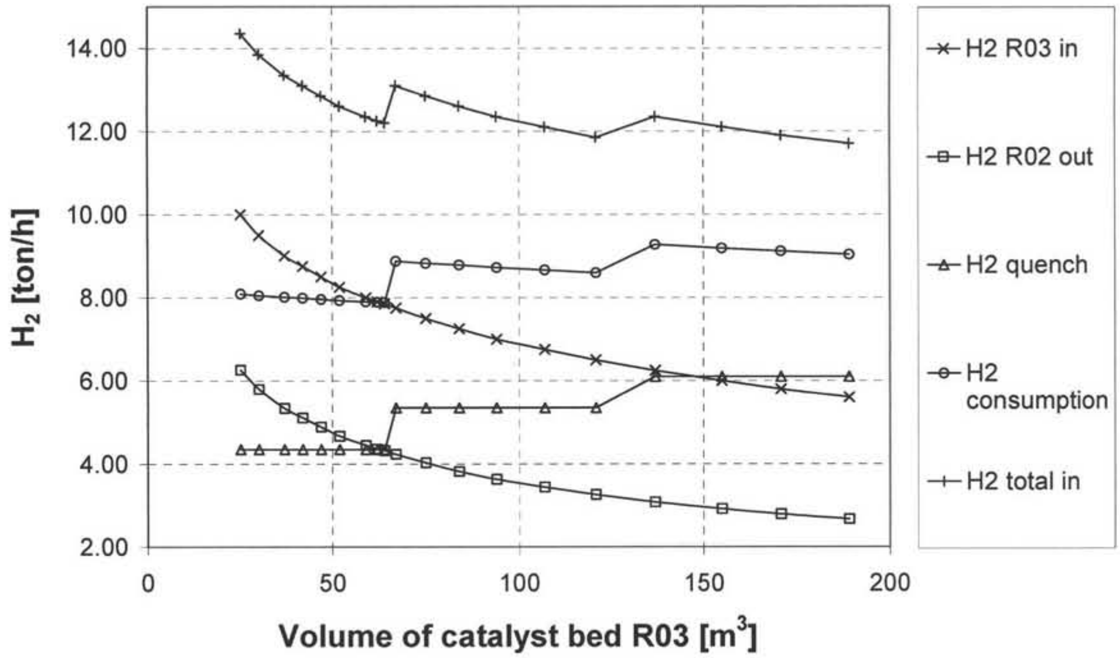


Figure 8.1: Hydrogen flows to and from (R03) and consumption as function of the volume of catalyst of (R03)

Table 8.3: Sensitivity analysis of the added hydrogen to the volume of the reactor (R03)

Sensitivity analysis of the added hydrogen and the R03 reactor volume					
V_{R03} [m^3 cat]	H_2 R03 in [ton/h]	H_2 quench [ton/h]	H_2 total in [ton/h]	H_2 R02 out [ton/h]	H_2 consumption [ton/h]
189	5.60	6.10	11.70	2.67	9.03
171	5.80	6.10	11.90	2.79	9.11
155	6.00	6.10	12.10	2.92	9.18
137	6.25	6.10	12.35	3.08	9.27
121	6.50	5.35	11.85	3.26	8.59
107	6.75	5.35	12.10	3.44	8.66
94	7.00	5.35	12.35	3.63	8.72
84	7.25	5.35	12.60	3.82	8.78
75	7.50	5.35	12.85	4.03	8.82
67	7.75	5.35	13.10	4.23	8.87
64	7.85	4.35	12.20	4.32	7.88
62	7.90	4.35	12.25	4.36	7.89
59	8.00	4.35	12.35	4.45	7.90
52	8.25	4.35	12.60	4.67	7.93
47	8.50	4.35	12.85	4.89	7.96
42	8.75	4.35	13.10	5.11	7.99
37	9.00	4.35	13.35	5.34	8.01
30	9.50	4.35	13.85	5.80	8.05
25	10.00	4.35	14.35	6.26	8.09
The optimal volume of R03 and H_2 addition regarding H_2 consumption					
V_{R03}	H_2 R03 in	H_2 quench	H_2 total in	H_2 R02 out	H_2 consumption
64	7.85	4.35	12.2	4.32	7.88

8.1.2.4 Conclusion of the Matlab ® simulation

The Distillate has a sulphur content of 47.5 ppm S, the hydrogen consumption is 7.88 t/h, the total hydrogen towards the reactor system is 12.20 t/h and the hydrogen to the recycle system is 4.32 t/h.

The Matlab ® simulation is based on provided component distributions for feed Distillate and GO-Finate. The hydrogen needed to convert the feed into the products was more then the hydrogen that is consumed in the current process, according to the heat and material balances. The sulphur content of the feed was also higher then mentioned in other provided information sources. Although the component distribution should be validated because of the mentioned differences, it was the best source of information to use for reactor design.

The reactor design is optimized for the minimum hydrogen consumption because hydrogen is the key factor in operation costs. The Distillate is just meeting the specification of 50 ppm S, so if catalyst activity is decreasing towards the end of run, more catalyst volume may be required.

The usage of hydrogen simulated in Aspen ® and Matlab ® differ but the recycle of hydrogen, important for the compressor and MEA-unit does not differ. As is mentioned the simulated hydrogen consumption is based on the component distribution, which should be validated.

8.2 Equipment selection and design

As was mentioned in 8.1.1 and from process flow sheet in 5.1 the following equipment is new compared to the current process:

- Pump: P01
- Reactor: (R03)
- Heat Exchangers: (E01), (E02)

The following equipment is not new. Only operation has changed.

- Exchangers: (E03), (E07), (E08), (E09), (E10)
- Compressor: (C01)
- Drums: (D01), (D02), (D04), (D05), (D07), (D08)
- Fractionator: (D03)

In agreement with the principal, only the new equipment is mentioned in detail. For the equipment that has changed only the changes will be mentioned. All equipment data sheets are included in 15.4 and 15.5.

9 Wastes

In every process there are wastes. These are classified as indirect wastes and direct wastes. Indirect wastes are caused by pollution occurring during manufacturing of feedstocks and plant equipment or as a result of product usage. For this report these wastes will not be considered.
Direct wastes originate directly from the designed plant. The process wastes are summarized in Table 9.1.

Table 9-1: Overview of process wastes and their causes and effects.

Waste	Cause	Effect/Remedy
Off-gas	Fractionator light gasses	The off-gas is sent to other parts of the plant, outside the battery limit. It will not be disposed directly into the environment.
Purge	Neccesary to control the flow through the compressor	The purge can be mixed with treat-gas, to prevent it from entering the environment directly.
Cooling water Process water	Equipment needs cooling. Water can become contaminated when pipes leak. Also process water is discharged from e.g. the compressor or the MEA unit.	This water needs to be cooled, purified or neutralized before it can be discharged into sewers.
Treat-gas recycle	The reacted gas can also be considered as waste.	The gas is treated in a flash-drum, to strip it from hydrocarbons and water. Then it is sent to an liquid-extractor unit, which removes H_2S. The gas is then recycled.
Sour water	Desulphurization reactions	Sour water is treated in a different plant, which produces sulphur. This sulphur is sold.
Hydrogensulphide in MEA	The recycle gas is treated in a liquid-extractor, which uses MEA as the solvent. The rich MEA contains H_2S	The H_2S is separated from the MEA and treated in the same plant as the sour water.
Spent Catalyst	Catalysts need to be changed every 1-$1^1/_2$ years for the main reactors and every 10 weeks for the guard reactor.	Catalysts are regenerated outside the plant site.

Wastes can also be caused by mis-operation. In case of an emergency off-specification product and unused reactants can be produced. There are several measures that can be taken to prevent mis-operation. The product can be reprocessed and the reactant can be recycled. Tight control systems, alarms and interlocks can be installed to reduce the risk of mis-operation. Also sample points, equipment drains and pumps should be sited so that any leaks flow into the plant effluent collection system and not into sewers.

Noise and visual impact are also considered as waste, but since the plant already exists, the added effect will be minimal.

10 Process safety

As in every design, attention has to be paid to safety. There are many methods available to assess the safety of a process, some less elaborate than others. From literature[14] these methods can be divided into four classes:

- Class 1: based solely on the properties of the materials used. For example: Flammability and reactivity.
- Class 2: takes the quantities of hazardous materials into account.

Class 1 and 2 together indicate the potential of a hazard.

- Class 3: includes penalties for hazardous operation, i.e. conditions which increase the potential for and probability of unwanted events (e.g. high pressures).
- Class 4: takes into account certain preventive and protective measures. The resulting hazard is that of after the plant has been modified.

For this report two methods are mandatory: HAZOP (Hazard And Operability Study) and the Fire and Explosion Index assessment from DOW, which are both class 3 methods. The HAZOP focuses on safety in operation in general and interactions between units. The DOW F&E Index focuses on fire and explosion risks.

Also some minor attention will be paid to the toxicity of components in the process. A class 1 method will be used here: the NFPA Material Factor.

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10.1 Toxicity

The American National Fire Protection Agency (NFPA) has developed a simple hazard index, which ranks hazards in 3 categories: Flammability, Reactivity and Health. Ratings (numbers) are assigned, which range from 0 (no hazard) to 4(maximum hazard). A more detailed explanation can be found in 15.3.1.

As can be seen from Table 15.6, H_2S, NH_2 and MEA have a rating of 3 or higher. This means that these components cause serious injury.

H_2S is a highly toxic and also flammable gas. As ammonia it has a MAC-value which is lower than 20 mg/m^3). H_2S is a key-compound in the process and extra care should be taken to prevent accidents that release this compound to the environment.

From the LD_{50} data it can also be seen that MEA is harmful, by comparing this data with the classification given in Table 15.7.

10.2 Fire and Explosion Index

A hazard classification has been made of the process according to the DOW fire and explosion index [15]. The detailed index for all units is shown in 15.3.2. For every unit a degree of hazard is calculated. Normally they are summarized in one sheet per unit, as in Table 15.9, where an example of an index sheet is given for the compressor.

From the table presented in the appendix it is clear that almost all units have an index between 1 and 24, which means a light hazard. The compressor has an index which is around 65, which means a moderate hazard. The compressor is the most hazardous unit in the process. Overall the process does not present any high risks.

The hazards are classified as in Table 10.1. The Fire and Explosion Index is ended by determining exposure areas. A summary sheet is presented Table 10.2. The explanation is as follows: The compressor represents a 62% damage probability to 381 m^2 of surrounding area, in the event of an accident.

Table 10.1: Degree of Hazard for Fire and Explosion index

1-60	light
61-96	Moderate
97-127	Intermediate
128-158	Heavy
159-up	Severe

Table 10.2: Example of Risk analysis summary sheet for the compressor

<table>
<tr><td colspan="4">Process Unit Risk Analysis</td></tr>
<tr><td>Area/Country:
South West Netherlands</td><td>Division:
-</td><td>Location
Rotterdam</td><td>Date
20-12-2006</td></tr>
<tr><td>Site
-</td><td>Manufacturing Unit
Go-Finer</td><td colspan="2">Process Unit
Compressor</td></tr>
<tr><td colspan="4">Materials in Process Unit
Acetaldehyde</td></tr>
<tr><td colspan="2">State of Operation</td><td colspan="2">Basic Materials for Material Factor
Light Hydrocarbons, Hydrogen</td></tr>
<tr><td colspan="2">1. Fire & Explosion Index (F&EI)</td><td>43</td><td>[-]</td></tr>
<tr><td colspan="2">2. Radius of Exposure</td><td>11</td><td>[m]</td></tr>
<tr><td colspan="2">3. Area of Exposure</td><td>381</td><td>[m^2]</td></tr>
<tr><td colspan="2">4. Value of Exposure</td><td></td><td>Mfl</td></tr>
<tr><td colspan="2">5. Damage Factor</td><td>0,62</td><td>[-]</td></tr>
</table>

10.3 HAZOP

The HAZOP has the advantage that it involves interaction of hazards between units. It is normally performed in a team of experts and is a very extensive operation. For this report, a 'reduced' HAZOP is done, which means that not all available guide-words will be used and only the following equipment will be considered: Reactor section, HPHS (D01), Fractionator (D03), Compressor (C01) and Pump 1 (P01). Only one flash-vessel is chosen, because all have the same function and about the same operating mode, except for pressure and temperatures.

The complete HAZOP can be found in 15.3.3.

10.4 Conclusions and recommendations concerning safety

Overall this process presents some risks because of the high operating pressure. Some components are hazardous and extra care should be taken to prevent these components from entering the environment.

Measures like tight control structures, clear emergency plans, frequent emergency exercises and dikes are not redundant.

11 Economy

In modifying an existing plant, simulations and calculations are required to get a proper design. But the design also needs to be economically profitable. Therefore the investment costs, annual production costs and the income should be determined. Once those major economic values are determined, economic criteria, costs review, sensitivities and negative cash flows can be calculated in order to get proper understanding of the design in an economic perspective.

In this chapter, the economic information for the design is given. Calculations and assumptions can be found in 15.6. All economic calculations are done according to [16].

11.1 Investment costs

For the calculation of the investment, the "Lang Method" is used [16]. As determined in chapter 5.1, the following new equipment will be used in the 'new' design: (1) Reactor 3 (R03); (2) Change of Reactor 2 (R02); (3) Heat-Exchanger 1 (E01); (4)E01; Heat-Exchanger 2 (E02) and (5) Pump 1 (P01). For those units, the Major Equipment Cost is calculated. This is multiplied by the "Lang-factors" for direct-costs for every unit, followed by multiplying with the "Lang-factors" for indirect-costs. Summation of the Fixed Capital Cost per Unit, will give the Total Investment Cost. How the "Lang-factors' are determined is explained in 15.6.1.1.

Table 11.1: Total investment cost with costs per unit (PCE: Major Equipment Cost, PPC: Physical Plant Cost, FCCU: Fixed Capital Cost per Unit).

Unit	PCE (k$)	"Lang-Factors" (direct cost)	PPC (k$)	"Lang-Factors" (indirect cost)	FCCU (k$)
Reactor 2 (R02)	398	1.10	437	1.45	634
Reactor 3 (R03)	262	2.55	667	1.45	967
Heat-Exchanger 1 (E01)	124	2.55	316	1.45	458
Heat-Exchanger 2 (E02)	124	2.55	316	1.45	458
Pump 1 (P01)	53	2.55	136	1.45	197
Total Investment Cost (k$)					**2.714**

11.2 Production Costs

The annual production (operating) costs are the costs which occur every year. The production costs are determined as deviation of the current process (so not the total operating costs are determined).

Table 11.2: Total annual production costs of the new design of the GO-finer (annual production costs are extra costs for the new design; current annual production costs are not included). [16]

Annual Production Costs		
Variable Costs	**k$/yr**	**Remarks:**
(1) Raw Materials	79.072	*See appendix XXX.2*
(2) Miscellaneous Materials	20	*10% of maintenance costs*
(3) Utilities	4.118	*See appendix XXX.2*
(4) Shipping and Packing	0	*usually negligable*
Sum-total A	83.210	*All variable costs*
Fixed Costs		
(5) Maintenance	204	*5-10% of fixed capital (see Table 11.1)*
(6) Operating Labour	0	*from manning estimates*
(7) Laboratory Costs	0	*20-23% of (6)*
(8) Supervision	0	*20% of (6)*
(9) Plant Overheads	0	*50% of (6)*
(10) Capital Charges	407	*15% of fixed capital (see Table 11.1)*
(11) Insurance	27	*1% of fixed capital (see Table 11.1)*
(12) Local Taxes	54	*2% of fixed capital (see Table 11.1)*
(13) Royalties	0	*1% of fixed capital (see Table 11.1)*
Sum-total B	692	*All fixed costs*
Direct Production Costs	83.902	*Sum-total A + Sum-total B*
(14) Sales Expense	20.976	*(14), (15) and (16) together is assumed to be 25% of Direct Production Cost*
(15) General Overheads		
(16) Research and Development		
Annual Production Costs	**878104.878**	
Production Cost ($/kg)	**0.16**	*(annual production cost/annual GO-finer Distillate produced)*

Remarks:

- Calculations of (1) raw materials costs and (3) utility costs, can be found in 15-86.
- The products of the GO-Finer (GO-Finate, Distillate, Naphta and other products) are feedstock for other processes on the ExxonMobil site. Therefore the shipping and packaging costs can be neglected.
- For the revamp of the existing GO-finer, no extra labour is required. Existing labour is sufficient to handle the changes in the process. In addition the operating labour (and therefore the laboratory costs, supervision and plant overheads) are equal to zero.
- The process used has exclusively been designed for ExxonMobil. Therefore no royalties and licence fees had to be paid and this factor will be equal to zero.

11.3 Income and Cash-Flow

The income of the products from the GO-finer can be determined from the economic values of GO-Finate, GO-Finer Distillate, Naphtha and Off-Gas. However, economical analysis is performed only for the changes in the process and assumes current costs constant. Those current costs are not taken into account for the economical analysis. This means that the current values of the products are also not taken into account.

By reducing the sulphur content in the Distillate stream to 50ppm and GO-Finate to 200 ppm, extra economic value is added to the streams. Also change in density of the GO-Finate stream gives extra economic value. The ratio of produced GO-Finate, Distillate and Naphtha is called the spread between them. This will also increase the economic value of the streams. In Table 11.3 the increase of the economic value is given.

Table 11.3: Extra economic value of products streams (source: ExxonMobil)

Stream	Action	Increase economic value
GO-Finer Distillate	S decrease to 50ppm	15 \$/t
GO-Finer Distillate	S decrease to 10ppm	20 \$/t
GO-Finate	S decrease	none
GO-Finate	Density decrease	1 \$/t per density point decrease
GO-Finate : GO-finer Distillate	Spread of streams	60 \$/t
GO-finer Distillate : Naphta	Spread of streams	30 \$/t

Remarks:

- The simulations as discussed in 8.2 predict the sulphur content in the Distillate to be 50ppm. Therefore the decrease to 10ppm is not taken into account.
- Because of (R03) the amount of mild hydro-cracking will be higher in comparison with the current GO-finer operation. Although the density of the GO-Finate stream will be lower, no absolute value is determined and therefore not considered in the economic analysis.
- The magnitude of the streams of the GO-Finate, Distillate and Naphtha are decided with the use of pseudo components in the simulation. Therefore the real spreading of those streams is not determined. Because a slight increase in hydro-cracking can be expected due to the extra reactor, the GO-Finate stream will be smaller and the Distillate and Naphtha stream will be larger in the new design. Exact values are not known and therefore not taken into account in the economic analysis.

The (extra) annual income of the new GO-finer design is determined with the use of the following formula:

(annual) income = increase economic value * mass flow Distillate * operating time

The total annual income is $9.6 \cdot 10^3$ k\$/yr.

It has to be mentioned that this income is fictive. The income is the extra value of the Distillate stream, but is not necessarily extra income from sale.
The "net cash-flow" at any time is the difference between the earning and expenditure of a system (difference between annual income and annual operating costs). In this design, the "net cash-flow" will be $-95*10 \cdot 10^3$ k\$/yr which means the design will cost the company 95Million dollars each year.

11.4 Economic Evaluation

The negative "net cash-flow" of this project is in economic perspective unfavourable. It means that the project will never pay back, but only cost extra money each year. With that in mind, it is useless to determine the Rate On Return (ROR), Pay Out Time (POT) and the Discounted Cash Flow Rate on Return (DCFROR=earning power). All of those economic values will be negative and has no more value than just an indication that the project cost money each year instead of making profit.

The investment costs of the project are small, in comparison with the annual operating costs. The main factor responsible for the high annual operating costs is the raw materials costs, of which the hydrogen consumption is the key factor. In order to make this project economically profitable, the use of hydrogen should be lowered significantly. But for deep desulphurization, more hydrogen is required, which makes it hard to reduce it. Even with increase of efficiency in the new design, the hydrogen consumption will still be large (in comparison with the current system).
It has to be mentioned that the purpose of deep desulphurization of the Distillate stream is not to make more profit; future legislation demands lower sulphur content of the Distillate stream. Adaptations of processes caused by new legislations will usually cost money, instead of making it more profitable. However, the extra costs should be as low as possible.

12 Creativity and group process tools

It was agreed with ExxonMobil that this chapter could be omitted. The creativity will be discussed with the group and creativity coach. As the content of this report is proprietary, the group coach will not read the report. Therefore, it is not necessary to have this topic in this report.

13 Conclusions

13.1 Conclusion

In this CPD project a revamp of a process has been performed to reduce the sulphur concentration in Distillate. This design has been worked out to some extent.
The current process produces Distillate, which contains 2500 ppm sulphur. The sulphur content needed to be reduced to 50 ppm, caused by expected changes in legislation. The current process is composed of:

- A reaction section of two reactors. One is a guard reactor, which removes contaminants (metals) and a second reactor, where desulphurization, denitrofication and mild hydrocracking reactions occur;
- A separation section for the vapour-stream, where the produced hydrogen sulphide (and ammonia) is removed;
- A separation section for the liquid-stream, where the products are separated.

After literature research process options have been proposed, from which one option was chosen.
The chosen option was to add an additional reactor to the current reaction section, which has the same catalysts and thus performs the same reactions. This reactor will be a fixed-bed reactor, with internals that separate vapour- and liquid-streams at the bottom of the reactor. The current reactor will need the same internals as well, in order to separate the vapour- and liquid-streams. The reactors will operate in semi-countercurrent mode, which means that the liquid goes from the current reactors to the new reactor and the vapour in reverse order.
The changes in the reaction section require changes in the separation sequence. The vapour from the second reactor demands separation of the hydrocarbons from the unreacted hydrogen (and formed hydrogen sulphide). The liquid from the third reactor is now sent directly to the LPHS. After the LPHS both the liquid and the vapour stream go through a heat exchanger.

A simulation was made in two programs: Matlab® to simulate the reactor section and Aspen® to simulate the rest of the process.
In Matlab® it was proven that the target of 50 ppm sulphur in the Distillate could be reached. For this an extensive simulation was written to calculate rate-constants. Also the volume of the new reactor and the extra hydrogen consumed could be determined.
In Aspen® was proven that the recycle is still within constraints. Also mass- and heat-balances were made using this program. Due to difficulties in the simulation these balances were not closing. Simulation in Aspen® is performed with the use of pseudo components and in Matlab® with real components.

An economic evaluation was performed. This proved however that this option is not economically profitable. The annual operating costs were too high, caused by the fact that much more hydrogen is needed for operation (hydrogen is very expensive). Adaptations caused by new legislation will usually cost money instead of making more profit.

Finally a safety analysis was done. The result of this was that the compressor presents the highest risks, caused by high pressure and hydrogen as medium. Hydrogen is an explosive gas. Also MEA, used in the extraction unit, proved to be a harmful liquid.
Measures were recommended to reduce risks.

13.2 Recommendations

Because the hydrogen consumption is the most important cost factor, the component distribution [7] provided by Exxon Mobil should be validated. The current use of hydrogen is significantly lower then what is calculated with the Matlab ® simulation based on the component distribution.

A further investigation about the use and possibilities of new and enhanced catalysts for the GO-finer unit might result in lower hydrogen consumption.

14 Literature

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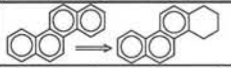
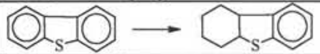
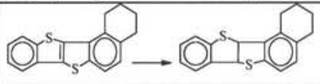
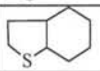
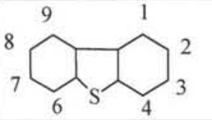
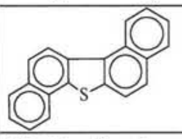
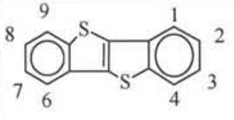
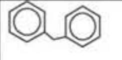
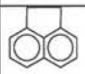
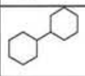
15 Appendices

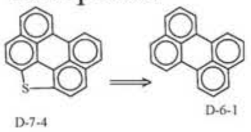
15.1 Thermodynamics and kinetics

Table 15.1: Proposed classification of reactions occurring in the reactor

Class	**Molecule**	**Group name**	**Initial estimation of rate**[a]
HYD of Aromatics:			
I		HYD of benzene-ring (no S)	
II		HYD of Benzene-ring (BT, DBT, DBDT)	
III		HYD of C-C bond (not cyclic)	
Desulphurization reactions			**Initial estimation of rate**[b] **[9]**
IV		thiophene (T)	
V		benzothiophene (BT)	>0.1 min^{-1}
VI		Dibenzothiophenes (DBT) without substituents	0.034-0.1 min^{-1}
VII		DBT with substituents at 4 OR 6 positions	0.013-0.34min^{-1}
VIII	Not in feed	DBT with substituents at 4 AND 6 positions	
IX		Dibenzo-di-thiophene (DBDT) And DBDT with substituents at 2 and/or 6 positions	
X	Not in feed	DBDT with substituents at 4 and/or 9 positions	
Cracking			
XI		aromatic C and non-aromatic C	
XII		C-C bond (not aromatic)	
XIII		C-C bond (between 2 cyclic carbons)	

Desulphurization occurs only with saturated molecules.
Cracking does not occur with sulphur containing molecules, only after desulphurization.
For simplicity: cyclic rings do not crack, this can be argued since these reactions have been observed.

Exceptions:



Molecule desulphurizes first, then HYD, because the sulphur is easily accessible.

15.1.1 Summary of Thermodynamic Information

Table 15.2: Summary of thermodynamic information obtained from principles

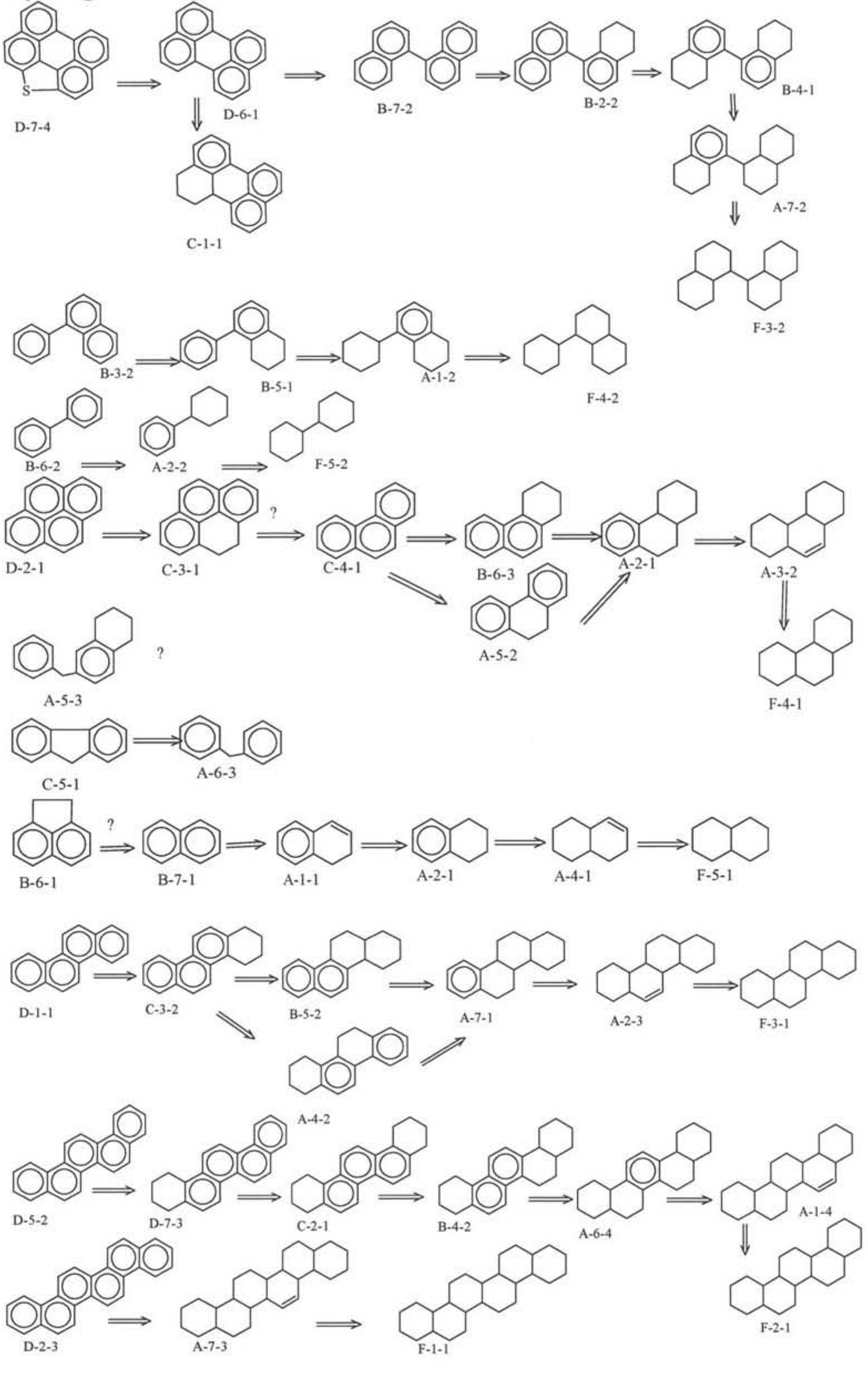
	S115 (feed to RX)	S116 (RX effluent)
T (^oC)	323	394
P (bar)	101	92.37
wt frac L	0.8320	0.5004
Enthalpy (MWatt)	-0.8638	-4.6655
C_p (kJ/kg K)		
Gas	5.2746	3.8708
Liquid	2.9187	3.2242
Compressability (z) of gas phase	1.0398	1.0330
Density (kg/m^3)		
Gas	16083.0204	29158.9873
liquid	727.2856	619.1355

Table 15.3: True boiling point curve (vol%) and required specifications (API gravity, temperature, pressure, density, flowrate and flashpoint) for feed and products (Naphtha, Distillate and GO-Finate)

Percent distilled	Temperature (^{o}C)			
	Feed	Naphtha	Distillate	GO-Finate
0	180	40	128	314
5	241	85	182	362
10	260	92	216	382
20	295	99	251	406
30	330	105	267	426
40	360	111	279	444
50	410	128	292	463
60	430	165	308	482
70	470	240	327	502
80	500	265	350	524
90	540	313	380	557
95	570	365	402	588
100	680	366	459	665
Specifications:				
Standard API gravity		47	28	16
Standard specific gravity (H_2O, 60F)		0.79	0.8858	0.9589
Temperature (^{O}C)	310	47	45	90
Pressure (bar)	100	6.5	8.7	6.6
Rate (t/hr)		3	78	54
Flash point (CC, ^{O}C)		-33	65	214

15.1.2 Proposed Reactions

Hydrogenation reaction:

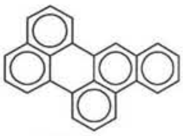


Miscellaneous components:

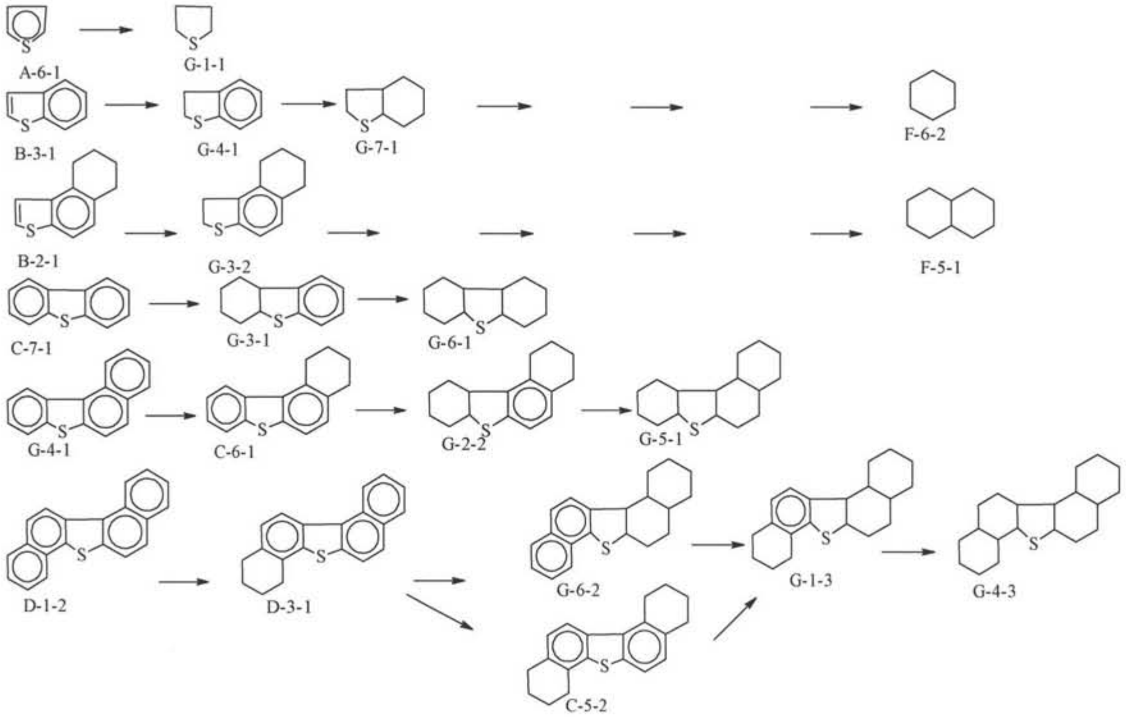

D-6-2

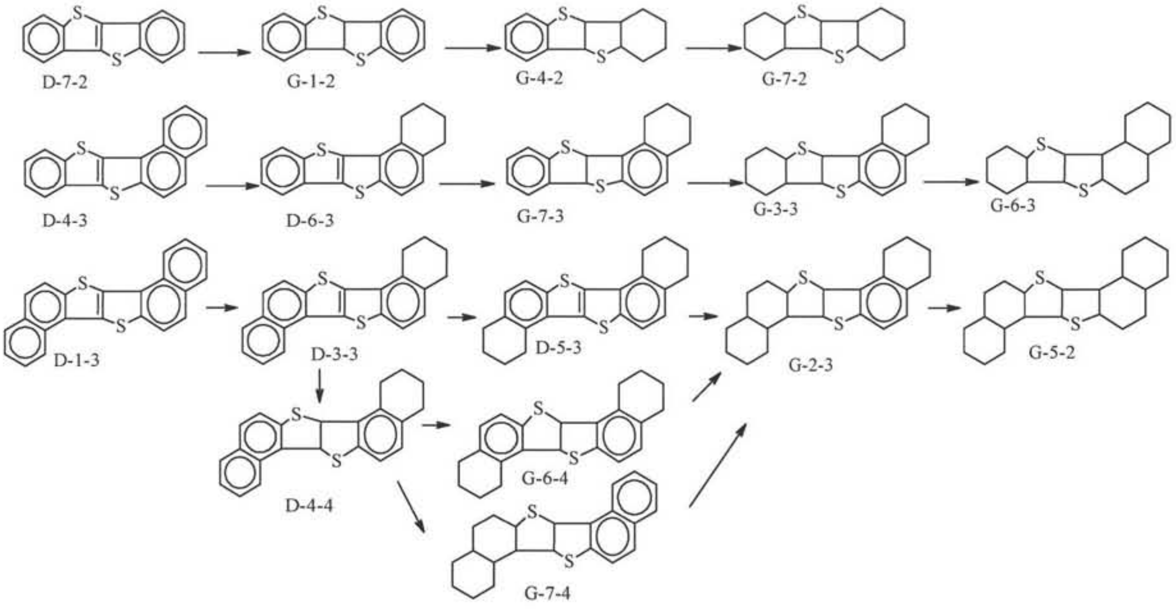

D-7-1


D-4-2

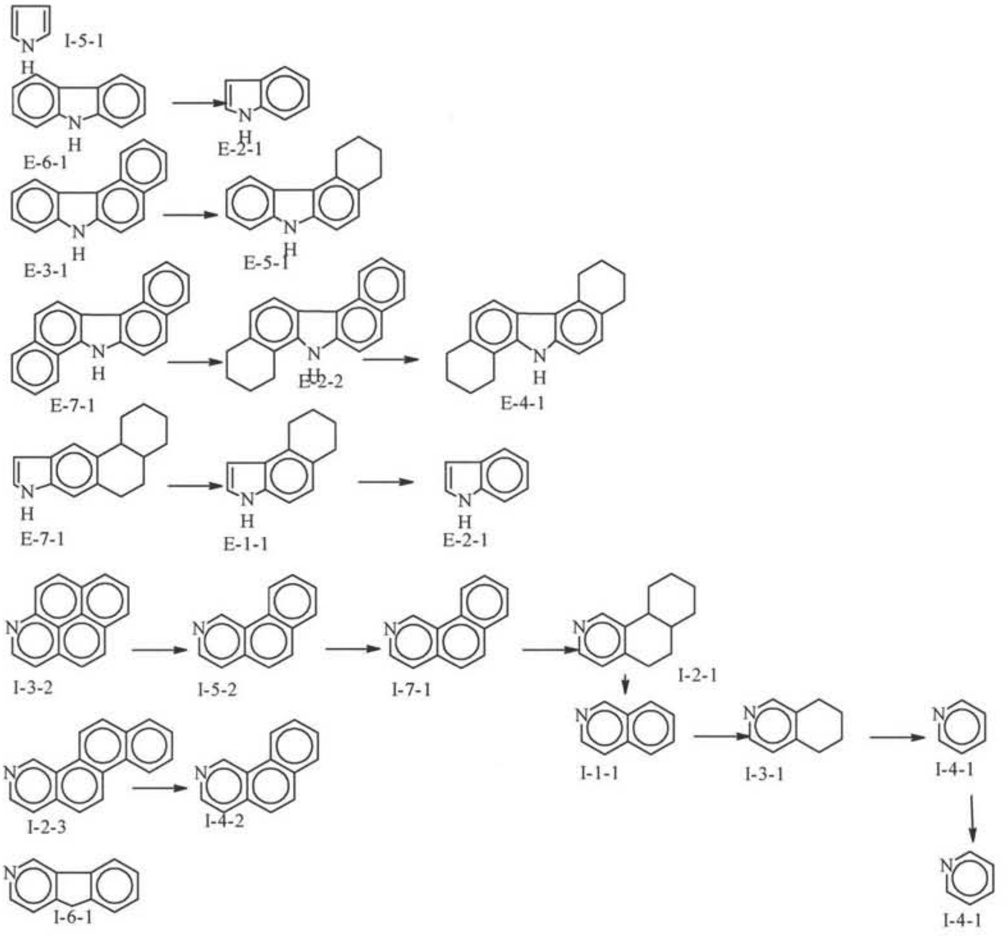

D-3-2

Hydrogenation of Sulphur containing components:



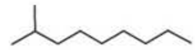


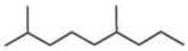
Hydrogenation of Nitrogen containing components:



Polairs


I-2-2
F-7-1


F-7-2

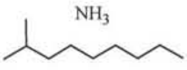

F-7-3


A-6-2

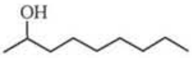

A-3-1


A-5-1

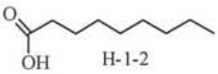

G-2-1



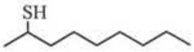
I-1-2



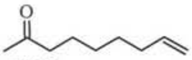
H-1-1



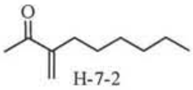
H-1-2



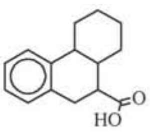
H-2-1



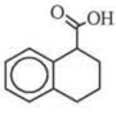
H-6-1



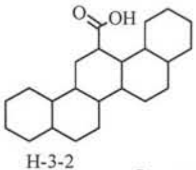
H-7-2



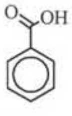
H-2-2



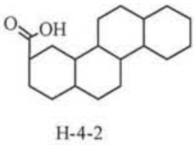
H-3-1



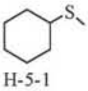
H-3-2



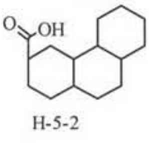
H-4-1



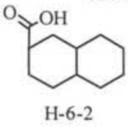
H-4-2



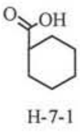
H-5-1



H-5-2



H-6-2



H-7-1

15.2 Stream summary

Stream nr	FEED,<S112>		<S113>		<S114>		<S115>		<S116V>		<S116L>		<S117>		<S118>		<S119>	
Name	Cold Feed		Heated feed from E01		Heated Feed from E02		Heated Feed from E03		Vapour from Reactor 2		Liquid from Reactor 2		Heated Vapour from Reactor 2 to D01		D01 Vapor Effluent		D01 Liquid Effluent	
Temperature (C)	250,00		287,49		308,17		350,76		400,00		400,00		318,00		300,00		300,00	
Pressure (bar)	110,00		110,00		110,00		110,00		90,00		90,00		90,00		90,00		90,00	
Vapour fraction	0,00		0,00		0,00		0,00		1,00		0,00		0,97		1,00		0,00	
Enthalpy (W)	-40425378,00		-36845338,00		-34802295,00		-30449309,00		-4155295,30		-23693199,00		-8508270,40		-5595726,80		-3871661,60	
Density (kg/m^3)	818,62		792,48		778,19		749,41		27,24		703,61		31,45		20,90		688,95	
Average MW	294,16		294,16		294,16		294,16		17,46		254,76		17,46		11,39		197,00	
Phase	LIQUID		LIQUID		LIQUID		LIQUID		VAPOR		LIQUID		MIXED		VAPOR		LIQUID	
COMPONENTS:	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/h
H2	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1963,25	3957,67	55,27	111,43	1963,25	3957,67	1956,06	3943,18	7,19	14,49
H20	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	49,78	896,83	0,36	6,47	49,78	896,83	49,60	893,59	0,18	3,24
MEA	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
NH3	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	41,42	705,36	3,26	55,51	41,42	705,36	40,77	694,32	0,65	11,0
C3	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	16,59	731,42	1,57	69,34	16,59	731,42	16,26	717,11	0,32	14,3
C1	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	155,85	2500,32	7,76	124,42	155,85	2500,32	154,62	2480,55	1,23	19,7
H2S	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	136,12	4639,07	11,24	383,17	136,12	4639,07	133,93	4564,71	2,18	74,3
C2	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	16,47	495,25	1,19	35,67	16,47	495,25	16,25	488,64	0,22	6,60
IC4	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	7,92	460,25	0,92	53,34	7,92	460,25	7,71	448,36	0,20	11,8
NC4	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	5,02	291,61	0,62	36,31	5,02	291,61	4,87	283,29	0,14	8,31
NC5	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	12,70	916,06	2,02	145,49	12,70	916,06	12,19	879,23	0,51	36,8
CYCLOPEN	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	10,60	743,11	2,00	140,61	10,60	743,11	10,07	706,50	0,52	36,6
ISOHEX	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	6,52	561,81	1,25	107,33	6,52	561,81	6,18	532,83	0,34	28,9
NC6	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	9,42	811,95	1,90	163,35	9,42	811,95	8,90	766,77	0,52	45,1
C02	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC185C	5,69	796,23	5,69	796,23	5,69	796,23	5,69	796,23	4,69	657,10	2,94	411,84	4,69	657,10	3,66	512,93	1,03	144,1
PC198C	7,97	1176,03	7,97	1176,03	7,97	1176,03	7,97	1176,03	6,29	927,92	4,45	656,15	6,29	927,92	4,72	695,62	1,57	232,3
PC212C	8,79	1374,14	8,79	1374,14	8,79	1374,14	8,79	1374,14	6,53	1020,74	5,31	830,24	6,53	1020,74	4,63	724,98	1,89	295,7
PC226C	10,06	1667,37	10,06	1667,37	10,06	1667,37	10,06	1667,37	6,96	1153,10	6,54	1083,18	6,96	1153,10	4,64	768,07	2,32	385,0
PC240C	12,83	2251,67	12,83	2251,67	12,83	2251,67	12,83	2251,67	8,15	1430,41	8,90	1562,32	8,15	1430,41	5,02	881,87	3,13	548,5
PC254C	29,58	5493,54	29,58	5493,54	29,58	5493,54	29,58	5493,54	17,06	3168,03	21,73	4035,96	17,06	3168,03	9,61	1784,37	7,45	1383,
PC267C	25,91	5066,04	25,91	5066,04	25,91	5066,04	25,91	5066,04	13,49	2638,96	19,93	3897,90	13,49	2638,96	6,89	1347,43	6,60	1291,
PC281C	25,70	5301,36	25,70	5301,36	25,70	5301,36	25,70	5301,36	11,90	2454,05	20,61	4251,33	11,90	2454,05	5,40	1113,12	6,50	1340,
PC295C	24,20	5259,72	24,20	5259,72	24,20	5259,72	24,20	5259,72	9,84	2140,01	20,09	4367,39	9,84	2140,01	3,90	847,91	5,94	1292,
PC309C	22,70	5196,81	22,70	5196,81	22,70	5196,81	22,70	5196,81	8,02	1837,19	19,41	4443,80	8,02	1837,19	2,72	623,89	5,30	1213,
PC323C	22,68	5463,25	22,68	5463,25	22,68	5463,25	22,68	5463,25	6,90	1661,43	19,87	4787,98	6,90	1661,43	1,97	474,58	4,93	1186,
PC337C	26,26	6653,22	26,26	6653,22	26,26	6653,22	26,26	6653,22	6,80	1723,11	23,50	5953,18	6,80	1723,11	1,60	405,90	5,20	1317,
PC350C	23,44	6221,64	23,44	6221,64	23,44	6221,64	23,44	6221,64	5,18	1374,09	21,32	5660,21	5,18	1374,09	1,00	265,35	4,18	1108,
PC364C	15,29	4258,29	15,29	4258,29	15,29	4258,29	15,29	4258,29	2,84	790,05	14,12	3932,01	2,84	790,05	0,44	121,84	2,40	668,2
PC378C	11,97	3496,12	11,97	3496,12	11,97	3496,12	11,97	3496,12	1,84	537,99	11,20	3270,70	1,84	537,99	0,22	64,71	1,62	473,2
PC392C	11,70	3580,07	11,70	3580,07	11,70	3580,07	11,70	3580,07	1,48	454,16	11,06	3386,62	1,48	454,16	0,14	42,00	1,35	412,1
PC406C	15,04	4824,73	15,04	4824,73	15,04	4824,73	15,04	4824,73	1,55	498,38	14,37	4608,66	1,55	498,38	0,11	34,67	1,45	463,7
PC420C	33,16	11104,62	33,16	11104,62	33,16	11104,62	33,16	11104,62	2,80	937,08	31,93	10691,42	2,80	937,08	0,15	49,05	2,65	888,0
PC439C	29,96	10642,04	29,96	10642,04	29,96	10642,04	29,96	10642,04	1,88	668,67	29,11	10340,33	1,88	668,67	0,06	23,01	1,82	645,6
PC470C	29,24	11362,94	29,24	11362,94	29,24	11362,94	29,24	11362,94	1,02	397,10	28,76	11175,84	1,02	397,10	0,01	5,62	1,01	391,4
PC495C	31,17	13031,25	31,17	13031,25	31,17	13031,25	31,17	13031,25	0,69	286,41	30,84	12892,75	0,69	286,41	0,00	2,07	0,68	284,3
PC523C	22,01	9911,95	22,01	9911,95	22,01	9911,95	22,01	9911,95	0,29	128,74	21,87	9848,09	0,29	128,74	0,00	0,44	0,28	128,3
PC549C	15,85	7631,74	15,85	7631,74	15,85	7631,74	15,85	7631,74	0,12	58,25	15,79	7602,17	0,12	58,25	0,00	0,09	0,12	58,1
PC578C	5,30	2738,43	5,30	2738,43	5,30	2738,43	5,30	2738,43	0,02	11,12	5,29	2732,65	0,02	11,12	0,00	0,01	0,02	11,1
PC607C	3,78	2082,97	3,78	2082,97	3,78	2082,97	3,78	2082,97	0,01	4,43	3,77	2080,61	0,01	4,43	0,00	0,00	0,01	4,43
PC635C	2,96	1735,30	2,96	1735,30	2,96	1735,30	2,96	1735,30	0,00	1,88	2,96	1734,28	0,00	1,88	0,00	0,00	0,00	1,88
PC664C	2,70	1678,52	2,70	1678,52	2,70	1678,52	2,70	1678,52	0,00	0,85	2,70	1678,04	0,00	0,85	0,00	0,00	0,00	0,85
TOTAL FLOW	475,93	140000,00	475,93	140000,00	475,93	140000,00	475,93	140000,00	2558,00	44671,97	507,73	129348,06	2558,00	44671,97	2474,33	28188,61	83,67	16483
m^3/hr	171,02		176,66		179,90		199,80		1820,42		196,38		1420,35		1494,72		28,02	
TBP Curve (C, vol%)																		
0%	188,21		188,21		188,21		188,21				-256,06						-257,18	
5%	240,67		240,67		240,67		240,67				198,48						105,54	
10%	261,05		261,05		261,05		261,05				255,63						223,14	
30%	329,70		329,70		329,70		329,70				334,72						271,54	
50%	409,45		409,45		409,45		409,45				414,73						307,42	
70%	469,29		469,29		469,29		469,29				474,66						345,54	
90%	537,39		537,39		537,39		537,39				540,18						423,02	
95%	571,23		571,23		571,23		571,23				575,01						453,96	
100%	651,35		651,35		651,35		651,35				653,04						513,41	

Stream nr	<S120>		<S121L>		<S121V>		<S124>		<S126L>		<S126V>		<S127>		<S128>		<S129>		<S130>	
Name	Mixed Liquid From R02		R03 Liquid Effluent		R03 Vapor Effluent		Steam for D07		D02 Liquid Effluent		D02 Vapor Effluent		Fractionator Liquid Feed from D02		Heated D02 Vapor		E10 Feed		E10 Effluent	
Temperature	388,98		390,00		390,00		43,00		400,00		400,00		348,55		350,00		165,44		46,00	
Pressure (bar)	90,00		110,00		110,00		100,00		3,00		3,00		5,00		3,00		90,00		90,00	
Vapour fraction	0,00		0,00		1,00		0,00		0,00		1,00		0,19		0,83		0,73		0,64	
Enthalpy (W)	-27564861,00		-25273737,00		-4114379,00		-87676662,00		-18366901,00		-4293413,70		-25508562,00		-6336456,90		-93272389,00		-102359384,00	
Density (kg/m^	696,45		705,57		26,93		995,40		715,48		8,20		185,35		10,50		43,60		65,19	
Average MW	246,59		249,31		14,02		18,02		346,13		146,97		290,13		146,97		13,44		13,44	
Phase	MIXED		LIQUID		VAPOR		LIQUID		LIQUID		VAPOR		MIXED		MIXED		MIXED		MIXED	
COMPONENTS:	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr
H2	62,46	125,92	65,15	131,33	1563,25	3151,32	0,00	0,00	0,37	0,75	64,77	130,58	0,37	0,75	64,77	130,58	1956,06	3943,18	1956,06	3943,18
H20	0,54	9,71	0,43	7,75	33,58	604,91	1110,17	20000,00	0,00	0,01	0,43	7,74	55,51	1000,01	0,43	7,74	1159,77	20893,59	1159,77	20893,59
MEA	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
NH3	3,91	66,55	3,27	55,67	26,94	458,73	0,00	0,00	0,06	0,95	3,21	54,72	0,06	0,95	3,21	54,72	40,77	694,32	40,77	694,32
C3	1,90	83,66	3,36	148,35	22,94	1011,41	0,00	0,00	0,07	3,08	3,29	145,27	0,07	3,08	3,29	145,27	16,26	717,11	16,26	717,11
C1	8,99	144,18	15,98	256,41	212,78	3413,61	0,00	0,00	0,17	2,68	15,82	253,73	0,17	2,68	15,82	253,73	154,62	2480,55	154,62	2480,55
H2S	13,42	457,53	5,26	179,23	41,34	1409,06	0,00	0,00	0,09	3,21	5,16	176,02	0,09	3,21	5,16	176,02	133,93	4564,71	133,93	4564,71
C2	1,41	42,28	0,98	29,50	8,90	267,47	0,00	0,00	0,02	0,46	0,97	29,04	0,02	0,46	0,97	29,04	16,25	488,64	16,25	488,64
IC4	1,12	65,24	1,40	81,39	7,75	450,51	0,00	0,00	0,04	2,10	1,36	79,30	0,04	2,10	1,36	79,30	7,71	448,36	7,71	448,36
NC4	0,77	44,62	1,24	72,07	6,37	370,10	0,00	0,00	0,03	2,00	1,21	70,08	0,03	2,00	1,21	70,08	4,87	283,29	4,87	283,29
NC5	2,53	182,33	2,31	166,78	9,22	665,27	0,00	0,00	0,08	5,98	2,23	160,80	0,08	5,98	2,23	160,80	12,19	879,23	12,19	879,23
CYCLOPEN	2,53	177,21	2,28	160,21	7,61	533,71	0,00	0,00	0,10	6,87	2,19	153,34	0,10	6,87	2,19	153,34	10,07	706,50	10,07	706,50
ISOHEX	1,58	136,31	1,64	141,35	5,40	465,62	0,00	0,00	0,07	6,16	1,57	135,19	0,07	6,16	1,57	135,19	6,18	532,83	6,18	532,83
NC6	2,42	208,53	2,55	220,03	7,96	686,16	0,00	0,00	0,12	10,11	2,44	209,93	0,12	10,11	2,44	209,93	8,90	766,77	8,90	766,77
C02	0,00	0,00	0.00	0,00	0,00	0,00	0,00	0,00	0,00	0.00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC185C	3,97	556,01	2,02	283,29	1,95	272,71	0,00	0,00	0,29	40,07	1,74	243,22	0,29	40,07	1,74	243,22	3,66	512,93	3,66	512,93
PC198C	6,02	888,46	3,26	480,41	2,77	408,06	0,00	0,00	0,52	75,99	2,74	404,41	0,52	75,99	2,74	404,41	4,72	695,62	4,72	695,62
PC212C	7,20	1125,99	4,15	649,14	3,05	476,85	0,00	0,00	0,75	116,56	3,40	532,58	0,75	116,56	3,40	532,58	4,63	724,98	4,63	724,98
PC226C	8,86	1468,20	5,43	899,28	3,43	568,91	0,00	0,00	1,11	183,32	4,32	715,96	1,11	183,32	4,32	715,96	4,64	768,07	4,64	768,07
PC240C	12,03	2110,86	7,80	1369,78	4,22	741,08	0,00	0,00	1,81	317,54	5,99	1052,24	1,81	317,54	5,99	1052,24	5,02	881,87	5,02	881,87
PC254C	29,19	5419,62	19,97	3709,11	9,21	1710,51	0,00	0,00	5,25	975,58	14,72	2733,53	5,25	975,58	14,72	2733,53	9,61	1784,37	9,61	1784,37
PC267C	26,54	5189,42	19,01	3718,55	7,52	1470,87	0,00	0,00	5,62	1098,62	13,40	2619,93	5,62	1098,62	13,40	2619,93	6,89	1347,43	6,89	1347,43
PC281C	27,11	5592,27	20,30	4188,22	6,81	1404,04	0,00	0,00	6,76	1394,07	13,55	2794,15	6,76	1394,07	13,55	2794,15	5,40	1113,12	5,40	1113,12
PC295C	26,03	5659,50	20,30	4411,78	5,74	1247,72	0,00	0,00	7,58	1648,38	12,71	2763,41	7,58	1648,38	12,71	2763,41	3,90	847,91	3,90	847,91
PC309C	24,71	5657,09	19,97	4572,88	4,74	1084,21	0,00	0,00	8,35	1910,96	11,63	2661,92	8,35	1910,96	11,63	2661,92	2,72	623,89	2,72	623,89
PC323C	24,80	5974,82	20,71	4988,64	4,09	986,19	0,00	0,00	9,63	2319,38	11,08	2669,25	9,63	2319,38	11,08	2669,25	1,97	474,58	1,97	474,58
PC337C	28,69	7270,39	24,66	6247,28	4,04	1023,11	0,00	0,00	12,68	3212,97	11,98	3034,31	12,68	3212,97	11,98	3034,31	1,60	405,90	1,60	405,90
PC350C	25,50	6768,96	22,44	5956,26	3,06	812,70	0,00	0,00	12,61	3346,92	9,83	2609,34	12,61	3346,92	9,83	2609,34	1,00	265,35	1,00	265,35
PC364C	16,52	4600,22	14,86	4136,43	1,67	463,79	0,00	0,00	9,09	2530,91	5,77	1605,52	9,09	2530,91	5,77	1605,52	0,44	121,84	0,44	121,84
PC378C	12,82	3743,98	11,75	3431,40	1,07	312,58	0,00	0,00	7,78	2272,39	3,97	1159,01	7,78	2272,39	3,97	1159,01	0,22	64,71	0,22	64,71
PC392C	12,41	3798,79	11,56	3538.06	0,85	260,73	0,00	0,00	8,21	2512,37	3,35	1025,68	8,21	2512,37	3,35	1025,68	0,14	42,00	0,14	42,00
PC406C	15,82	5072,37	14,94	4790,05	0,88	282,32	0,00	0,00	11,29	3620,89	3,65	1169,16	11,29	3620,89	3,65	1169,16	0,11	34,67	0,11	34,67
PC420C	34,58	11579,45	33,01	11055,54	1,56	523,91	0,00	0,00	26,27	8796,53	6,75	2259,01	26,27	8796,53	6,75	2259,01	0,15	49,05	0,15	49,05
PC439C	30,93	10985,99	29,89	10619,01	1,03	366,99	0,00	0,00	25,24	8965,98	4,65	1653,02	25,24	8965,98	4,65	1653,02	0,06	23,01	0,06	23,01
PC470C	29,76	11567,32	29,22	11357,30	0,54	210,02	0,00	0,00	26,66	10361,12	2,56	996,19	26,66	10361,12	2,56	996,19	0,01	5,62	0,01	5,62
PC495C	31,52	13177,09	31,17	13029,16	0,35	147,93	0,00	0,00	29,47	12319,00	1,70	710,15	29,47	12319,00	1,70	710,15	0,00	2,07	0,00	2,07
PC523C	22,16	9976,39	22,01	9911,51	0,14	64,88	0,00	0,00	21,32	9600,84	0,69	310,67	21,32	9600,84	0,69	310,67	0,00	0,44	0,00	0,44
PC549C	15,91	7660,33	15,85	7631,65	0,06	28,68	0,00	0,00	15,57	7496,04	0,28	135,60	15,57	7496,04	0,28	135,60	0,00	0,09	0,00	0,09
PC578C	5,31	2743,76	5,30	2738,42	0,01	5,33	0,00	0,00	5,25	2713,78	0,05	24,65	5,25	2713,78	0,05	24,65	0,00	0,01	0,00	0,01
PC607C	3,78	2085,04	3,78	2082,97	0,00	2,07	0,00	0,00	3,76	2073,66	0,02	9,31	3,76	2073,66	0,02	9,31	0,00	0,00	0,00	0,00
PC635C	2,97	1736,15	2,96	1735,30	0,00	0,85	0,00	0,00	2,96	1731,58	0,01	3,72	2,96	1731,58	0,01	3,72	0,00	0,00	0,00	0,00
PC664C	2,70	1678,90	2,70	1678,52	0,00	0,38	0,00	0,00	2,70	1676,93	0,00	1,59	2,70	1676,93	0,00	1,59	0,00	0,00	0,00	0,00
TOTAL FLOW	591,40	145831,43	524,89	130860,02	2022,84	28365,30	1110,17	20000,00	269,72	93356,76	255,17	37503,26	325,22	94356,76	255,17	37503,26	3584,49	48188,61	3584,49	48188,61
m^3/hr	209,39		185,47		1053,48		20,09		130,48		4573,04		509,06		3571,89		1105,15		739,16	
TBP Curve (C, vol%)																				
0%									225,72				225,72							
5%									287,02				287,02							
10%									319,99				319,99							
30%									408,88				408,88							
50%									451,98				451,98							
70%									500,43				500,43							
90%									557,76				557,76							
95%									598,81				598,81							
100%									660,91				660,91							

Stream nr	<S131>		<S132>		<S133>		<S134>		<S135>		<S136>		<S137>		<S138>		<S139>		<S
Name	Vapor effluent from D07 to D08		Sour Water from D07		Hydrocarbons from D07		D08 overhead to C01		C01 Feed		C01 Effluent Compressed Treat-gas		Frac Feed from D02 Vapor		Frac Top Out to E07		Cooled Frac Top Out from E07		O
Temperature	46,00		46,00		46,00		43,89		43,89		71,80		371,98		201,62		45,00		45,00
Pressure (bar)	88,00		88,00		88,00		80,00		80,00		110,00		3,00		3,00		3,00		3,00
Vapour fractio	1,00		0,00		0,00		0,89		0,89		1,00		0,66		1,00		0,11		1,00
Enthalpy (W)	-5555773,70		-91210606,00		-5590135,30		-23669169,00		-23669169,00		-3820001,00		-6566621,50		-44278363,00		-61069883,00		-1716375,
Density (kg/m	18,60		993,63		787,01		18,56		18,56		14,97		33,98		5,18		62,31		2,39
Average MW	5,78		18,02		114,55		5,64		5,64		4,09		148,87		65,73		65,73		20,89
Phase	VAPOR		LIQUID		LIQUID		MIXED		MIXED		VAPOR		MIXED		VAPOR		MIXED		VAPOR
COMPONENTS	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/h
H2	1951,12	3933,22	0,00	0,00	4,94	9,95	1756,01	3539,90	1756,01	3539,90	1756,01	3539,90	64,78	130,58	65,60	132,23	65,60	132,23	70,03
H20	3,63	65,47	1155,75	20821,18	0,39	6,94	252,06	4540,85	252,06	4540,85	7,47	134,60	0,89	15,98	463,57	8351,40	463,57	8351,40	3,94
MEA	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
NH3	34,64	590,00	0,00	0,00	6,13	104,32	0,42	7,15	0,42	7,15	0,42	7,15	3,21	54,73	4,46	75,96	4,46	75,96	1,95
C3	13,28	585,63	0,00	0,00	2,98	131,47	11,95	527,07	11,95	527,07	11,95	527,07	3,29	145,28	8,22	362,62	8,22	362,62	5,81
C1	151,99	2438,29	0,00	0,00	2,63	42,27	136,79	2194,46	136,79	2194,46	136,79	2194,46	15,82	253,73	16,92	271,45	16,92	271,45	18,51
H2S	118,42	4035,89	0,00	0,00	15,52	528,82	1,29	43,94	1,29	43,94	1,29	43,94	5,17	176,04	13,92	474,33	13,92	474,33	19,73
C2	15,08	453,40	0,00	0,00	1,17	35,25	13,57	408,06	13,57	408,06	13,57	408,06	0,97	29,04	1,53	46,01	1,53	46,01	2,09
IC4	5,18	301,05	0,00	0,00	2,53	147,30	4,66	270,95	4,66	270,95	4,66	270,95	1,36	79,31	7,67	445,87	7,67	445,87	3,24
NC4	2,98	172,95	0,00	0,00	1,90	110,34	2,68	155,66	2,68	155,66	2,68	155,66	1,21	70,09	7,78	452,12	7,78	452,12	2,41
NC5	4,31	310,83	0,00	0,00	7,88	568,40	3,88	279,75	3,88	279,75	3,88	279,75	2,23	160,84	46,03	3321,43	46,03	3321,43	5,33
CYCLOPEN	2,64	185,24	0,00	0,00	7,43	521,26	2,38	166,72	2,38	166,72	2,38	166,72	2,19	153,40	52,88	3708,71	52,88	3708,71	4,09
ISOHEX	1,30	112,16	0,00	0,00	4,88	420,67	1,17	100,94	1,17	100,94	1,17	100,94	1,57	135,25	40,56	3495,25	40,56	3495,25	2,20
NC6	1,50	129,62	0,00	0,00	7,39	637,15	1,35	116,66	1,35	116,66	1,35	116,66	2,44	210,02	67,50	5816,73	67,50	5816,73	2,73
C02	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC185C	0,01	1,95	0,00	0,00	3,65	510,98	0,00	0,00	0,00	0,00	0,00	0,00	1,75	244,38	52,25	7313,97	52,25	7313,97	0,03
PC198C	0,01	1,64	0,00	0,00	4,70	693,97	0,00	0,00	0,00	0,00	0,00	0,00	2,77	407,93	72,78	10737,09	72,78	10737,09	0,02
PC212C	0,01	0,99	0,00	0,00	4,63	723,99	0,00	0,00	0,00	0,00	0,00	0,00	3,49	546,24	74,91	11717,81	74,91	11717,81	0,01
PC226C	0,00	0,59	0,00	0,00	4,63	767,48	0,00	0,00	0,00	0,00	0,00	0,00	4,68	776,00	56,11	9297,59	56,11	9297,59	0,01
PC240C	0,00	0,38	0,00	0,00	5,02	881,50	0,00	0,00	0,00	0,00	0,00	0,00	6,79	1192,07	18,21	3195,56	18,21	3195,56	0,00
PC254C	0,00	0,41	0,00	0,00	9,61	1783,96	0,00	0,00	0,00	0,00	0,00	0,00	16,47	3059,01	6,89	1278,73	6,89	1278,73	0,00
PC267C	0,00	0,17	0,00	0,00	6,89	1347,26	0,00	0,00	0,00	0,00	0,00	0,00	14,71	2875,94	1,53	300,16	1,53	300,16	0,00
PC281C	0,00	0,08	0,00	0,00	5,40	1113,04	0,00	0,00	0,00	0,00	0,00	0,00	14,62	3015,82	0,57	117,90	0,57	117,90	0,00
PC295C	0,00	0,03	0,00	0,00	3,90	847,87	0,00	0,00	0,00	0,00	0,00	0,00	13,54	2943,47	0,25	53,87	0,25	53,87	0,00
PC309C	0,00	0,01	0,00	0,00	2,72	623,88	0,00	0,00	0,00	0,00	0,00	0,00	12,26	2805,98	0,11	25,37	0,11	25,37	0,00
PC323C	0,00	0,00	0,00	0,00	1,97	474,57	0,00	0,00	0,00	0,00	0,00	0,00	11,58	2790,60	0,05	12,57	0,05	12,57	0,00
PC337C	0,00	0,00	0,00	0,00	1,60	405,90	0,00	0,00	0,00	0,00	0,00	0,00	12,44	3151,28	0,03	7,01	0,03	7,01	0,00
PC350C	0,00	0,00	0,00	0,00	1,00	265,35	0,00	0,00	0,00	0,00	0,00	0,00	10,16	2696,13	0,01	3,05	0,01	3,05	0,00
PC364C	0,00	0,00	0,00	0,00	0,44	121,84	0,00	0,00	0,00	0,00	0,00	0,00	5,93	1651,55	0,00	0,91	0,00	0,91	0,00
PC378C	0,00	0,00	0,00	0,00	0,22	64,71	0,00	0,00	0,00	0,00	0,00	0,00	4,07	1187,65	0,00	0,31	0,00	0,31	0,00
PC392C	0,00	0,00	0,00	0,00	0,14	42,00	0,00	0,00	0,00	0,00	0,00	0,00	3,42	1047,54	0,00	0,13	0,00	0,13	0,00
PC406C	0,00	0,00	0,00	0,00	0,11	34,67	0,00	0,00	0,00	0,00	0,00	0,00	3,71	1190,44	0,00	0,06	0,00	0,06	0,00
PC420C	0,00	0,00	0,00	0,00	0,15	49,05	0,00	0,00	0,00	0,00	0,00	0,00	6,85	2293,87	0,00	0,06	0,00	0,06	0,00
PC439C	0,00	0,00	0,00	0,00	0,06	23,01	0,00	0,00	0,00	0,00	0,00	0,00	4,71	1671,30	0,00	0,01	0,00	0,01	0,00
PC470C	0,00	0,00	0,00	0,00	0,01	5,62	0,00	0,00	0,00	0,00	0,00	0,00	2,57	997,19	0,00	0,00	0,00	0,00	0,00
PC495C	0,00	0,00	0,00	0,00	0,00	2,07	0,00	0,00	0,00	0,00	0,00	0,00	1,70	710,52	0,00	0,00	0,00	0,00	0,00
PC523C	0,00	0,00	0,00	0,00	0,00	0,44	0,00	0,00	0,00	0,00	0,00	0,00	0,69	310,75	0,00	0,00	0,00	0,00	0,00
PC549C	0,00	0,00	0,00	0,00	0,00	0,09	0,00	0,00	0,00	0,00	0,00	0,00	0,28	135,62	0,00	0,00	0,00	0,00	0,00
PC578C	0,00	0,00	0,00	0,00	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,05	24,65	0,00	0,00	0,00	0,00	0,00
PC607C	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,02	9,31	0,00	0,00	0,00	0,00	0,00
PC635C	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01	3,72	0,00	0,00	0,00	0,00	0,00
PC664C	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	1,59	0,00	0,00	0,00	0,00	0,00
TOTAL FLOW	2306,11	13320,02	1155,75	20821,18	122,63	14047,40	2188,20	12352,09	2188,20	12352,09	1943,62	7945,85	264,36	39354,85	1080,35	71016,26	1080,35	71016,26	142,
m^3/hr	715,95		20,95		17,85		665,68		665,68		530,88		1158,17		13702,90		1139,66		1243,
TBP Curve (C, vol%)																			
0%					-254,35														
5%					-62,87														
10%					-33,53														
30%					89,88														
50%					234,01														
70%					265,93														
90%					312,02														
95%					335,76														
100%					382,10														

Stream nr	<S141>		<S142>		<S143>		<S144>		<S145A>		S145B		S146A		S146B		<S150>		<S162>	
Name	Sour Water Frac		Naphta Product		Frac Reflux		Reflux Frac Distillate		D06 Effluent to E09		Go-Finer Distillate		Frac Bottom to E08		Go-Finate Product		Treat-gas R03		Purge	
Temperature (C)	45,00		45,94		45,94		357,84		357,84		90,00		457,64		46,00		64,48			
Pressure (bar)	3,00		3,00		3,00		2,70		2,70		2,70		3,00		3,00		100,00			
Vapour fraction	0,00		0,00		0,00		1,00		0,00		0,00		0,00		0,00		0,99			
Enthalpy (W)	-35026671,00		-3004960,40		-27044677,00		-230163,20		-15230154,00		-28243634,00		-9443449,00		-25697790,00		-6748412,70			
Density (kg/m^3)	966,32		775,89		775,89		11,48		673,28		890,45		718,71		999,40		12,61			
Average MW	18,00		120,49		120,49		201,52		250,77		250,77		414,50		414,50		3,68			
Phase	LIQUID		MIXED		MIXED		VAPOR		LIQUID		LIQUID		LIQUID		LIQUID		MIXED			
COMPONENTS	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr
H2	0,00	0,00	0,05	0,10	0,45	0,91	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	3330,03	6712,93	0,00	0,00
H20	438,74	7904,09	2,13	38,32	19,14	344,86	0,46	8,24	0,03	0,56	0,03	0,56	0,04	0,65	0,04	0,65	30,87	556,22	0,00	0,00
MEA	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
NH3	7,31	124,56	0,13	2,25	1,19	20,29	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,29	5,01	0,00	0,00
C3	0,00	0,00	0,54	23,81	4,86	214,28	0,00	0,01	0,00	0,01	0,00	0,01	0,00	0,00	0,00	0,00	15,35	676,95	0,00	0,00
C1	0,00	0,01	0,10	1,67	0,94	15,04	0,00	0,01	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	179,75	2883,61	0,00	0,00
H2S	0,09	2,95	0,96	32,79	8,66	295,11	0,00	0,01	0,00	0,01	0,00	0,01	0,00	0,00	0,00	0,00	0,90	30,76	0,00	0,00
C2	0,00	0,00	0,06	1,83	0,55	16,51	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	24,86	747,64	0,00	0,00
IC4	0,00	0,00	0,70	40,50	6,27	364,49	0,00	0,01	0,00	0,01	0,00	0,01	0,00	0,00	0,00	0,00	4,59	266,66	0,00	0,00
NC4	0,00	0,00	0,73	42,23	6,54	380,06	0,00	0,01	0,00	0,01	0,00	0,01	0,00	0,00	0,00	0,00	4,26	247,56	0,00	0,00
NC5	0,00	0,00	4,86	350,52	43,72	3154,71	0,00	0,05	0,00	0,06	0,00	0,06	0,00	0,01	0,00	0,01	3,46	249,72	0,00	0,00
CYCLOPEN	0,00	0,01	5,62	394,29	50,60	3548,60	0,00	0,06	0,00	0,09	0,00	0,09	0,00	0,01	0,00	0,01	1,66	116,70	0,00	0,00
ISOHEX	0,00	0,00	4,32	372,67	38,92	3354,00	0,00	0,05	0,00	0,09	0,00	0,09	0,00	0,01	0,00	0,01	0,82	70,66	0,00	0,00
NC6	0,00	0,00	7,22	621,87	64,95	5596,87	0,00	0,09	0,00	0,16	0,00	0,16	0,00	0,01	0,00	0,01	8,10	697,66	0,00	0,00
C02	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC185C	0,00	0,00	5,59	782,10	50,28	7038,92	0,01	1,17	0,06	7,77	0,06	7,77	0,00	0,47	0,00	0,47	0,00	0,00	0,00	0,00
PC198C	0,00	0,00	7,75	1142,77	69,71	10284,92	0,02	3,52	0,18	27,15	0,18	27,15	0,01	1,08	0,01	1,08	0,00	0,00	0,00	0,00
PC212C	0,00	0,00	7,95	1243,98	71,58	11195,86	0,09	13,66	0,80	125,13	0,80	125,13	0,01	2,06	0,01	2,06	0,00	0,00	0,00	0,00
PC226C	0,00	0,00	6,07	1006,42	54,67	9057,81	0,36	60,04	3,96	655,47	3,96	655,47	0,02	4,00	0,02	4,00	0,00	0,00	0,00	0,00
PC240C	0,00	0,00	2,32	407,69	20,90	3669,28	0,80	139,83	10,45	1834,88	10,45	1834,88	0,05	8,57	0,05	8,57	0,00	0,00	0,00	0,00
PC254C	0,00	0,00	1,65	306,26	14,84	2756,36	1,75	325,49	27,76	5154,31	27,76	5154,31	0,17	32,39	0,17	32,39	0,00	0,00	0,00	0,00
PC267C	0,00	0,00	0,84	164,74	7,58	1482,67	1,31	256,01	24,84	4856,92	24,84	4856,92	0,23	44,14	0,23	44,14	0,00	0,00	0,00	0,00
PC281C	0,00	0,00	0,60	123,09	5,37	1107,85	1,07	221,67	24,77	5109,96	24,77	5109,96	0,33	68,21	0,33	68,21	0,00	0,00	0,00	0,00
PC295C	0,00	0,00	0,41	90,17	3,73	811,57	0,83	180,07	23,33	5071,56	23,33	5071,56	0,45	97,93	0,45	97,93	0,00	0,00	0,00	0,00
PC309C	0,00	0,00	0,28	64,93	2,55	584,33	0,63	144,05	21,81	4994,12	21,81	4994,12	0,60	137,73	0,60	137,73	0,00	0,00	0,00	0,00
PC323C	0,00	0,00	0,20	48,71	1,82	438,43	0,50	121,35	21,63	5212,00	21,63	5212,00	0,84	202,51	0,84	202,51	0,00	0,00	0,00	0,00
PC337C	0,00	0,00	0,16	41,29	1,47	371,61	0,46	116,97	24,75	6272,04	24,75	6272,04	1,34	339,86	1,34	339,86	0,00	0,00	0,00	0,00
PC350C	0,00	0,00	0,10	26,84	0,91	241,56	0,33	86,79	21,74	5770,64	21,74	5770,64	1,60	424,13	1,60	424,13	0,00	0,00	0,00	0,00
PC364C	0,00	0,00	0,04	12,27	0,40	110,47	0,17	46,04	13,86	3858,32	13,86	3858,32	1,39	387,67	1,39	387,67	0,00	0,00	0,00	0,00
PC378C	0,00	0,00	0,02	6,50	0,20	58,52	0,10	28,64	10,49	3065,91	10,49	3065,91	1,45	423,70	1,45	423,70	0,00	0,00	0,00	0,00
PC392C	0,00	0,00	0,01	4,21	0,12	37,92	0,07	21,86	9,82	3004,73	9,82	3004,73	1,87	571,13	1,87	571,13	0,00	0,00	0,00	0,00
PC406C	0,00	0,00	0,01	3,47	0,10	31,26	0,07	21,28	11,87	3807,03	11,87	3807,03	3,16	1014,22	3,16	1014,22	0,00	0,00	0,00	0,00
PC420C	0,00	0,00	0,01	4,91	0,13	44,20	0,10	34,85	24,08	8062,94	24,08	8062,94	9,07	3036,76	9,07	3036,76	0,00	0,00	0,00	0,00
PC439C	0,00	0,00	0,01	2,30	0,06	20,72	0,05	18,27	17,27	6133,88	17,27	6133,88	12,68	4505,85	12,68	4505,85	0,00	0,00	0,00	0,00
PC470C	0,00	0,00	0,00	0,56	0,01	5,06	0,00	1,00	1,82	705,63	1,82	705,63	27,42	10656,75	27,42	10656,75	0,00	0,00	0,00	0,00
PC495C	0,00	0,00	0,00	0,21	0,00	1,87	0,00	0,37	1,11	465,11	1,11	465,11	30,06	12565,92	30,06	12565,92	0,00	0,00	0,00	0,00
PC523C	0,00	0,00	0,00	0,04	0,00	0,39	0,00	0,08	0,44	196,30	0,44	196,30	21,58	9715,61	21,58	9715,61	0,00	0,00	0,00	0,00
PC549C	0,00	0,00	0,00	0,01	0,00	0,08	0,00	0,02	0,17	84,22	0,17	84,22	15,67	7547,51	15,67	7547,51	0,00	0,00	0,00	0,00
PC578C	0,00	0,00	0,00	0,00	0,00	0,01	0,00	0,00	0,03	15,16	0,03	15,16	5,27	2723,27	5,27	2723,27	0,00	0,00	0,00	0,00
PC607C	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01	5,70	0,01	5,70	3,77	2077,27	3,77	2077,27	0,00	0,00	0,00	0,00
PC635C	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	2,27	0,00	2,27	2,96	1733,03	2,96	1733,03	0,00	0,00	0,00	0,00
PC664C	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,97	0,00	0,97	2,70	1677,55	2,70	1677,55	0,00	0,00	0,00	0,00
TOTAL FLOW	446,14	8031,61	61,47	7406,36	553,24	66657,36	9,19	1851,59	297,09	74501,14	297,09	74501,14	144,75	60000,00	144,75	60000,00	3604,95	13262,09	0,00	0,00
m^3/hr	8,31		9,55		85,91		161,24		110,65		83,67		83,48		60,04		1051,38		0,00	
TBP Curve (C, vol%)																				
0%			-56,01		-56,01		208,75		220,44		220,44		302,20		302,20					
5%			28,15		28,15		233,85		249,44		249,44		399,15		399,15					
10%			47,40		47,40		242,75		259,20		259,20		422,56		422,56					
30%			108,77		108,77		260,94		297,80		297,80		472,11		472,11					
50%			198,99		198,99		280,30		336,59		336,59		498,03		498,03					
70%			217,13		217,13		308,42		381,17		381,17		528,27		528,27					
90%			249,92		249,91		353,49		426,17		426,17		584,06		584,06					
95%			275,06		275,06		385,12		444,47		444,47		624,68		624,68					
100%			334,96		334,96		425,22		481,12		481,12		667,49		667,49					

Stream nr	<S165>		<S154>		<S167>		<S169>		<S160>		<S161>		<S162>		<S163>		<S164>		L-MEA		R-MEA	
Name	Liquid Feed R03		E02 Effluent		Steam to D02 Effluent		Steam to Frac bottom		Liquid Effluent D04		Distillate Frac Out		Make-Up Gas		Total Treat-gas feed		Treat-gas R02		Lean MEA		Rich MEA	
Temperature (C)	390,00		350,00		344,00		300,00		45,00		321,13		60,00		64,48		64,48		40,00		43,89	
Pressure (bar)	110,00		3,00		8,00		10,00		3,00		3,00		100,00		100,00		100,00		80,00		80,00	
Vapour fraction	0,00		0,00		1,00		1,00		0,00		0,00		0,99		0,99		0,99		0,00		0,07	
Enthalpy (W)	-27412793,00		-21946976,00		-3561617,80		-25121427,00		-30049673,00		-17697577,00		-5820604,90		-9640589,40		-2892176,80		-246141920,00		-228335746,00	
Density (kg/m^3)	703,30		758,66		2,85		3,88		787,43		707,69		11,95		12,61		12,61		997,19		528,68	
Average MW	246,59		346,13		18,02		18,02		120,49		249,29		3,43		3,68		3,68		26,91		26,24	
Phase	LIQUID		MIXED		VAPOR		VAPOR		LIQUID		LIQUID		MIXED		MIXED		MIXED		LIQUID		MIXED	
COMPONENTS	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr	kmol/hr	kg/hr
H2	62,47	125,92	0,37	0,75	0,00	0,00	0,00	0,00	0,50	1,01	0,00	0,00	3001,17	6050,00	4757,18	9589,90	1427,15	2876,97	0,00	0,00	195,11	393,32
H2O	0,54	9,71	0,00	0,01	55,51	1000,00	388,56	7000,00	21,27	383,18	0,49	8,80	36,64	660,00	44,11	794,60	13,23	238,38	2516,92	45343,00	2268,50	40867,62
MEA	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	654,84	4000,00	654,84	4000,00
NH3	3,91	66,55	0,06	0,95	0,00	0,00	0,00	0,00	1,32	22,55	0,00	0,01	0,00	0,00	0,42	7,15	0,13	2,15	7,34	125,00	41,56	707,85
C3	1,90	83,66	0,07	3,08	0,00	0,00	0,00	0,00	5,40	238,08	0,00	0,03	9,98	440,00	21,93	967,07	6,58	290,12	0,00	0,00	1,33	58,56
C1	8,99	144,18	0,17	2,68	0,00	0,00	0,00	0,00	1,04	16,71	0,00	0,01	119,99	1925,00	256,78	4119,45	77,03	1235,83	0,00	0,00	15,20	243,83
H2S	13,42	457,53	0,09	3,21	0,00	0,00	0,00	0,00	9,62	327,89	0,00	0,02	0,00	0,00	1,29	43,94	0,39	13,18	10,50	358,00	127,63	4349,95
C2	1,41	42,28	0,02	0,46	0,00	0,00	0,00	0,00	0,61	18,35	0,00	0,00	21,95	660,00	35,52	1068,06	10,66	320,42	0,00	0,00	1,51	45,34
IC4	1,12	65,24	0,04	2,10	0,00	0,00	0,00	0,00	6,97	404,98	0,00	0,02	1,89	110,00	6,55	380,95	1,97	114,28	0,00	0,00	0,52	30,11
NC4	0,77	44,62	0,03	2,00	0,00	0,00	0,00	0,00	7,27	422,29	0,00	0,02	3,41	198,00	6,08	353,66	1,83	106,10	0,00	0,00	0,30	17,30
NC5	2,53	182,33	0,08	5,98	0,00	0,00	0,00	0,00	48,58	3505,25	0,00	0,10	1,07	77,00	4,94	356,75	1,48	107,02	0,00	0,00	0,43	31,08
CYCLOPEN	2,53	177,21	0,10	6,87	0,00	0,00	0,00	0,00	56,22	3942,89	0,00	0,15	0,00	0,00	2,38	166,72	0,71	50,01	0,00	0,00	0,26	18,52
ISOHEX	1,58	136,31	0,07	6,16	0,00	0,00	0,00	0,00	43,24	3726,66	0,00	0,14	0,00	0,00	1,17	100,94	0,35	30,28	0,00	0,00	0,13	11,22
NC6	2,42	208,53	0,12	10,11	0,00	0,00	0,00	0,00	72,16	6218,73	0,00	0,26	10,21	880,00	11,57	996,66	3,47	299,00	0,00	0,00	0,15	12,96
CO2	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC185C	3,97	556,01	0,29	40,07	0,00	0,00	0,00	0,00	55,87	7821,02	0,06	8,93	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01	1,95
PC198C	6,02	888,46	0,52	75,99	0,00	0,00	0,00	0,00	77,46	11427,66	0,21	30,67	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01	1,64
PC212C	7,20	1126,00	0,75	116,56	0,00	0,00	0,00	0,00	79,53	12439,81	0,89	138,81	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01	0,99
PC226C	8,86	1468,21	1,11	183,32	0,00	0,00	0,00	0,00	60,74	10064,26	4,32	715,60	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,59
PC240C	12,03	2110,87	1,81	317,54	0,00	0,00	0,00	0,00	23,23	4076,96	11,25	1974,63	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,38
PC254C	29,19	5419,65	5,25	975,58	0,00	0,00	0,00	0,00	16,49	3062,70	29,51	5479,80	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,41
PC267C	26,54	5189,46	5,62	1098,63	0,00	0,00	0,00	0,00	8,42	1647,44	26,15	5112,93	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,17
PC281C	27,11	5592,28	6,76	1394,07	0,00	0,00	0,00	0,00	5,97	1230,96	25,85	5331,63	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,08
PC295C	26,04	5659,53	7,58	1648,38	0,00	0,00	0,00	0,00	4,15	901,76	24,16	5251,64	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,03
PC309C	24,71	5657,12	8,35	1910,96	0,00	0,00	0,00	0,00	2,84	649,26	22,44	5138,18	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,01
PC323C	24,80	5974,86	9,63	2319,39	0,00	0,00	0,00	0,00	2,02	487,16	22,14	5333,36	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC337C	28,69	7270,44	12,68	3212,98	0,00	0,00	0,00	0,00	1,63	412,91	25,22	6389,02	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC350C	25,50	6769,00	12,61	3346,93	0,00	0,00	0,00	0,00	1,01	268,40	22,07	5857,42	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC364C	16,52	4600,24	9,09	2530,92	0,00	0,00	0,00	0,00	0,44	122,75	14,02	3904,35	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC378C	12,82	3744,00	7,78	2272,40	0,00	0,00	0,00	0,00	0,22	65,02	10,59	3094,53	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC392C	12,41	3798,80	8,21	2512,38	0,00	0,00	0,00	0,00	0,14	42,13	9,89	3026,56	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC406C	15,82	5072,39	11,29	3620,90	0,00	0,00	0,00	0,00	0,11	34,73	11,94	3828,28	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC420C	34,58	11579,49	26,27	8796,55	0,00	0,00	0,00	0,00	0,15	49,11	24,18	8097,73	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC439C	30,93	10986,03	25,24	8966,00	0,00	0,00	0,00	0,00	0,06	23,03	17,32	6152,33	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC470C	29,76	11567,34	26,66	10361,13	0,00	0,00	0,00	0,00	0,01	5,63	1,82	706,66	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC495C	31,52	13177,11	29,47	12319,02	0,00	0,00	0,00	0,00	0,00	2,07	1,11	465,50	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC523C	22,16	9976,40	21,32	9600,85	0,00	0,00	0,00	0,00	0,00	0,44	0,44	196,38	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC549C	15,91	7660,33	15,57	7496,05	0,00	0,00	0,00	0,00	0,00	0,09	0,17	84,24	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC578C	5,31	2743,76	5,25	2713,78	0,00	0,00	0,00	0,00	0,00	0,01	0,03	15,16	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC607C	3,78	2085,04	3,76	2073,66	0,00	0,00	0,00	0,00	0,00	0,00	0,01	5,70	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC635C	2,97	1736,15	2,96	1731,58	0,00	0,00	0,00	0,00	0,00	0,00	0,00	2,27	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
PC664C	2,70	1678,90	2,70	1676,93	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,97	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00	0,00
TOTAL FLOW	591,40	145831,95	269,72	93356,89	55,51	1000,00	388,56	7000,00	614,71	74063,86	306,28	76352,87	3206,30	11000,00	5149,92	18945,84	1544,98	5683,75	3189,60	85826,00	3307,51	86793,93
m^3/hr	207,35		123,06		350,74		1805,82		94,06		107,89		920,44		1501,97		450,59		86,07		164,17	
TBP Curve (C, vol%)																						
0%			225,72						-56,01		219,56											
5%			287,02						28,15		248,89											
10%			319,99						47,40		258,42											
30%			408,88						108,77		296,14											
50%			451,98						198,99		335,14											
70%			500,43						217,13		379,01											
90%			557,76						249,92		425,85											
95%			598,81						275,06		443,67											
100%			660,91						334,96		480,33											

15.3 Safety

15.3.1 NFPA Material factor

An explanation of the ratings is given in Table 15.4. Since flammability and reactivity are already covered by the DOW index, only Health will be elaborated on here.

Table 15.4: National Fire Protection Agency (NFPA) rating system for Flammability, Reactivity and Health [14]

Flammability(f)	N_f	Reactivity (r)	N_r	Health (h)	Nh
Non-combustable	0	Non-reactive even under fire	0	No hazard beyond that of ordinary combustibles	0
Flash point >100°C	1	Mildly reactive, upon heating and pressure	1	Only minor injury likely	1
40°C <flash point >100°C	2	Significantly reactive without heating	2	Medical attention required to avoid temporary or residual injury	2
20°C <flash point >40°C	3	Detonation possible with confinement	3	Materials causing serious injury	3
Flash point >20°C	4	Detonation possible without confinement	4	Short exposure causes death or serious injury.	4

The NFPA values are based on measurable properties. For health they are based on MAC-values. The Dutch Pressure Vessel Code grades the rating according to the MAC-values, shown in Table 15.5.

In 3.4 a pure components summary is given. It contains some MAC-values for components in the process. These are copied to Table 15.6 where also the health rating is assigned. Also some LD_{50} data is given. These can be compared with Table 15.7.

Table 15.5: Health rating estimate according to the Dutch Pressure Vessel Code[14]

MAC-value (in mg/m^3	Health-rating (N_h)
MAC>100	0
50<MAC<100	1
20<MAC<50	2
5<MAC<20	3
1<MAC<5	4
MAC<1	5

Table 15.6: Health rating of components in the process

Component Name	MAC Value (mg/m^3)	N_h	LD_{50} (oral,rat,mg/kg)
H_2O		0	
H_2			
C1			
C2			
H_2S	15	3	
NH_3	14	3	
C3			
IC4			
Butene			
NC4	1430	0	
IC5			
Pentene			
NC5	1800	0	
Cyclopentane			
Isohexane	720	0	
Hexene			
NC6	90	1	28710
Benzene	30	2	3800
Cyclohexane	300 ppm	1	29820
MEA	2,5	4	1720
CO2	9000	0	
Heavy Aromats			
Heavy S-components			
Heavy N-components			
Naphtha			

Table 15.7: Classification of LD_{50} values of chemicals

Category	LD_{50}, oral in rat, mg/kg	LD_{50}, dermal in rat or rabbit, mg/kg
Very Toxic	<25	<50
Toxic	25-200	50-400
Harmful	200-2000	400-2000

15.3.2 DOW Fire and Explosion index

Table 15.8: Fire and Explosion Index for Go-Finer. All indexes are determined per unit.

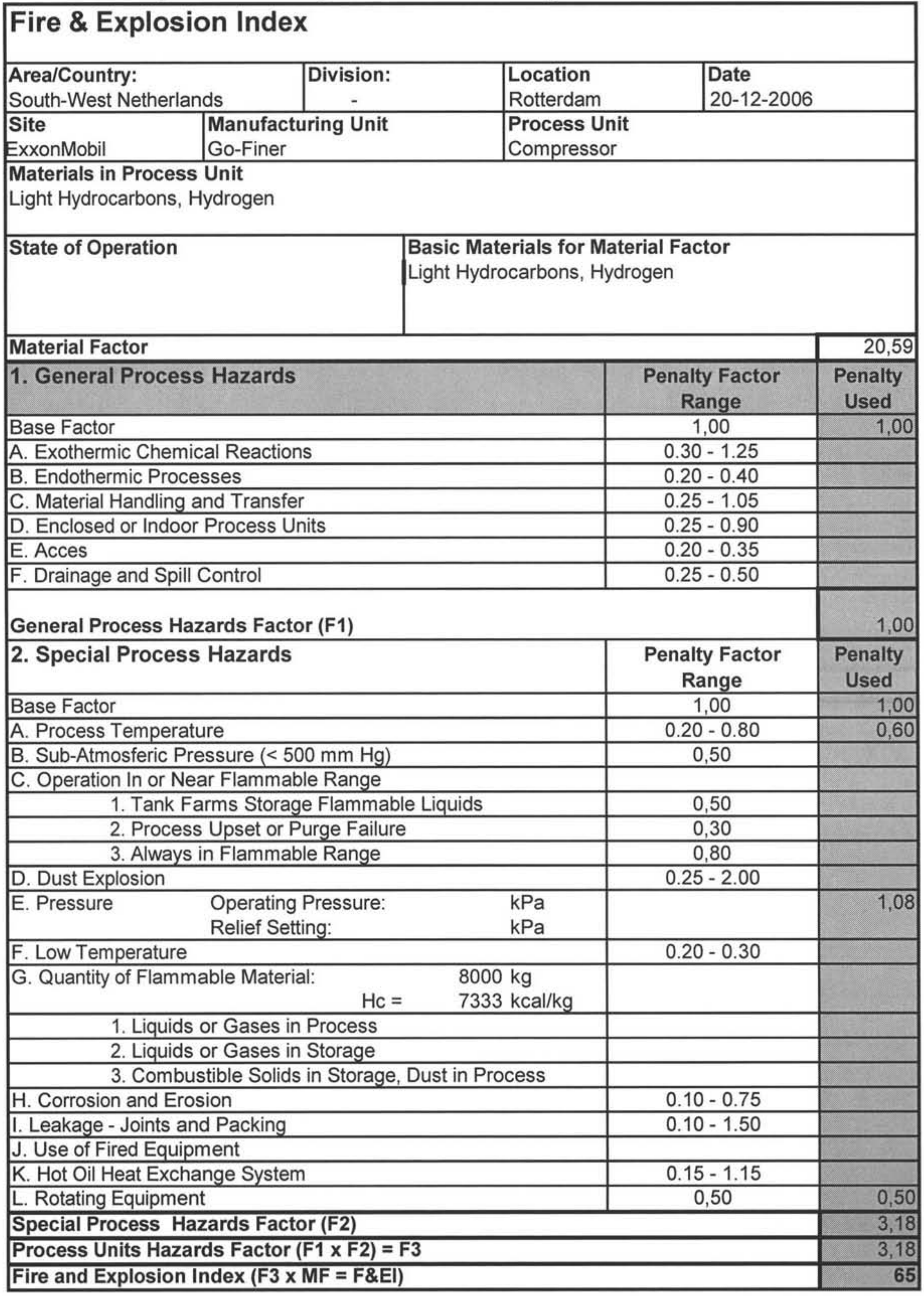
Unit	T	Pfluid	[illegible]	hydrofeed amount	Enthalpie stroom (kJ/s)	Enthalpie stroom (BTU/s)	[illegible] stroom per uur (10^6 BTU/s)	Material Factor MF	General process hazards Base Factor	A	B	C	D	E	F	General Process Hazard Factor F1
R1	377,492	95,5	100	[illegible]	[illegible]	[illegible]	[illegible]	2,16	1	0,3						1,3
R2	389,411	95	100	[illegible]	[illegible]	[illegible]	[illegible]	2,16	1	0,3						1,3
HPHS (D-8XX)	344	91	91,9	[illegible]	[illegible]	[illegible]	[illegible]	3,76	1							1
LPCSD (D-8XX)	323	8	8,19	[illegible]	[illegible]	[illegible]	[illegible]	0,25	1							1
FRACTIONATOR (T-8XX)	391	3,1	3,19	[illegible]	[illegible]	[illegible]	[illegible]	2,21	1							1
Frac OVERHEAD D-8XX	35	1,2	1,22	[illegible]	[illegible]	[illegible]	[illegible]	2,93	1							1
FRAC SIDESTREAM STRIPPER (T-8XX)	259	3	3,08	[illegible]	[illegible]	[illegible]	[illegible]	0,01	1							1
HPCS (D-8XX)	49	90	91,8	[illegible]	[illegible]	[illegible]	[illegible]	0,83	1							1
RECYCLE GAS SCRUBBER (T-8XX)	66	88	90,7	[illegible]	[illegible]	[illegible]	[illegible]	20,14	1							1
RECYCLE GAS COMPRESSOR (C-8XX)	55-70	90-100	91,6-110	[illegible]	[illegible]	[illegible]	[illegible]	20,9	1							1

Unit	Special process hazards Base Factor	A-1	A-2	A-3	B	C-1	C-2	C-3	D	E	F-1	G-1	G-2	G-3	H	I	J	K	L	Special Process Hazard Factor F2	Unit Hazard Factor F3=F1*F2	F&EI =F3*MF	Damage Factor	Exposure radius (m)
R1	1	0	0,6	0						0,82										2,62	3,276	7,07	0,5	2,4384
R2	1,00	0	0,6	0						0,82										2,62	3,276	7,07	0,5	2,4384
HPHS (D-8XX)	1,00	0,00	0,60	0,75						0,9										3,25	3,25	12,29	0,6	2,7432
LPCSD (D-8XX)	1,00	0,00	0,60	0,00						0,35										1,95	1,95	0,49	0	0
FRACTIONATOR (T-8XX)	1,00	0,00	0,60	0,75						0,1										2,45	2,45	5,37	0,2	1,524
Frac OVERHEAD D-8XX	1,00	0,00	0,00	0,00						0	0,15									1,15	1,15	3,38	0,1	0
FRAC SIDESTREAM STRIPPER (T-8XX)	1,00	0,00	0,00	0,00						0,1										1,1	1,1	0,00	0	0
HPCS (D-8XX)	1,00	0,00	0,60	0,00						0,9	0,4									2,9	2,9	2,84	0,15	6,096
RECYCLE GAS SCRUBBER (T-8XX)	1,00	0,00	0,60	0,00						0,9										2,5	2,5	51,60	0,47	12,065
RECYCLE GAS COMPRESSOR (C-8XX)	1,00	0,00	0,60	0,00						1,08									0,5	3,18	3,18	65,4	0,52	0,868

The material factor is determined by using lists provided by [15]. For components that are not listed, estimation can be made using flash points or boiling points.

An example of an index sheet is given in Table 15.9. The meaning of the letters is also given in Table 15.9. Points H through L are not considered, because of a lack of information on these subjects.

Table 15.9: Example of Fire and Explosion Index for the compressor



Fire & Explosion Index

Area/Country: South-West Netherlands	**Division:** -	**Location** Rotterdam	**Date** 20-12-2006
Site ExxonMobil	**Manufacturing Unit** Go-Finer	**Process Unit** Compressor	
Materials in Process Unit Light Hydrocarbons, Hydrogen			
State of Operation	**Basic Materials for Material Factor** Light Hydrocarbons, Hydrogen		

Material Factor		20,59
1. General Process Hazards	**Penalty Factor Range**	**Penalty Used**
Base Factor	1,00	1,00
A. Exothermic Chemical Reactions	0.30 - 1.25	
B. Endothermic Processes	0.20 - 0.40	
C. Material Handling and Transfer	0.25 - 1.05	
D. Enclosed or Indoor Process Units	0.25 - 0.90	
E. Acces	0.20 - 0.35	
F. Drainage and Spill Control	0.25 - 0.50	
General Process Hazards Factor (F1)		1,00
2. Special Process Hazards	**Penalty Factor Range**	**Penalty Used**
Base Factor	1,00	1,00
A. Process Temperature	0.20 - 0.80	0,60
B. Sub-Atmosferic Pressure (< 500 mm Hg)	0,50	
C. Operation In or Near Flammable Range		
1. Tank Farms Storage Flammable Liquids	0,50	
2. Process Upset or Purge Failure	0,30	
3. Always in Flammable Range	0,80	
D. Dust Explosion	0.25 - 2.00	
E. Pressure Operating Pressure: kPa Relief Setting: kPa		1,08
F. Low Temperature	0.20 - 0.30	
G. Quantity of Flammable Material: 8000 kg Hc = 7333 kcal/kg		
1. Liquids or Gases in Process		
2. Liquids or Gases in Storage		
3. Combustible Solids in Storage, Dust in Process		
H. Corrosion and Erosion	0.10 - 0.75	
I. Leakage - Joints and Packing	0.10 - 1.50	
J. Use of Fired Equipment		
K. Hot Oil Heat Exchange System	0.15 - 1.15	
L. Rotating Equipment	0,50	0,50
Special Process Hazards Factor (F2)		3,18
Process Units Hazards Factor (F1 x F2) = F3		3,18
Fire and Explosion Index (F3 x MF = F&EI)		65

15.3.3 HAZOP

Table 15.10: HAZOP of the revamped GO-Finer (1)

Number	Guideword	Parameter	Cause	Consequence	Action
Reactor section (R01,(R02), (R03)	no	Flow	1. No hydrocarbons available at the feed storage tank (not in process chosen, but in current process)	Loss of feed to reaction section, reduced output	(a) Ensure good communications with storage tank operators or (b) install low level alarm setting
			3. Line blockage, or valve closed	As in 1	Covered by (b)
			4. Line fracture	As in 1 Hydrocarbons discharged into environment	(c) Institute regular patrolling and inspections of lines
		Reaction	5. Not enough Hydrogen	Product not on spec	(d) Install flow controllers (e) Recirculate of product
			6. Temperature to low	As in 5	(e) Install high level alarm
	More	Temperature	7. Not enough quench	Higher pressures in lines	Covered by (e)
			8. Local insufficient mixing	Risk of reaction runaways	Covered by (e)
		Pressure	9. Higher reactor hold up		Covered by (e)
			10. Valve failure		Covered by (d)
	Less	Temperature	11. To much quench Not enough reaction	Less reaction, product not on spec	Covered by (e)
HPHS (D01)	Part of	Phase	12. Temperature to high/low	To much hydrocarbons in recycle	Install temperature controllers

Table 15.11: HAZOP of revamped GO-Finer (2)

Number	Guideword	Parameter	Cause	Consequence	Action
Compressor	More	Pressure	13. Higher feed pressure, due to cooling failure or flow-control failure	Rapture of pipes or equipment down stream at too high pressures	Safety relief valves should be installed to depressurize at too high pressures
		Flow	14. Failure of flow-control	Too large flows downstream, reaction and separation can be upset, product specifications may not be met	Purge with Safety relief valve if possible or regulate stream with other control structures. Repair flow control.
	less	Pressure	15. Lower feed pressure, due to high pressure drops upstream, or leakage of pipes	Product specifications not met due to low hydrogen pressure in reactor system. If leakage: loss of valuable materials and exposure to flammable materials	Unit shutdown, remove (partial) blockage casing high pressure drop (renew catalyst bed), closure of leakage.
		Flow	16. Leakage in pipe upstream	Plant exposed to flammable material and loss of valuable materials	Unit shutdown, closure of leakage
Fractionator	no	Flow	17. Power failure	Pump stops, reflux fails, separation is upset and vapour stream enlarged.	Use safety relief valve to get rid of extra vapour, stop feed to fractionator (probably GO-finer shutdown)
			18. Steam failure	No stripping steam, separation is upset because of disappearance vapour stream, products off spec, GO-Finate is larger	Use safety relief valves to send products (off spec) to blown down system, or if down stream processing can handle the products just repair steam failure

	More	Temperature	19. Condenser or cooler failure	At too high temperatures equipment can be damaged and vapour pressures can become too high which result in rapture/damage of equipment	Safety relief valve to get rid of over pressure, shutdown fractionator if condenser or other cooler fails, products will be off spec. unless fractionator can still operate within specs.
		Flow	20. Failure of up stream equipment or control structures	If additional load cannot be handled, flooding will occur, equipment damage and/or leakage of flammable materials can be consequence	Send additional load to blowdown/flare system if fractionator can not handle the load.
	less	Temperature	21. Temperature controller fails, too much cooling	Products will be off spec if temperature is too low	If the off spec is unacceptable send products to blowdown system or store reprocess it again.
		Flow	22. Failures upstream either control structure or leakage	If flow is too low trays can dry up, damage to equipment. Leakage of flammable materials can cause fire and explosion	If fractionator is drying up shut it down, if there is a leakage more has to be shutdown to stop leakage

15.4 Equipment Summary Sheets

In the following equipment summary sheets, the equipment in italic is not new. Therefore information provided is limited.

Equipment nr: **Name:**	(R03) Reactor	*(D03)* *Fractionator*	*(D01)* *HPHS*	*(D02)* *LPHS*	*(D04)* *Frac. Overhead drum*	*(D05)* *Frac. Side-stripper*	*(D07)* *HPCS*	*(D08)* *MEA-unit*
Pressure [bar]:	100	*3^{1}*	*90*	*3*	*3*	*2.7*	*88*	*88*
Temp. [°C]:	390	*187^{1}* *490^{2}*	*300*	*400*	*45*	*358*	*46*	*46*
Heat Duty (kW)			*960*	*2613*	*1327,9*	*2837.8*	*2.8*	
Volume [m^3]: **Diameter [m]:** **L or H [m]:**	70.4 3.00 10.0							
Internals - **Tray Type:** - **Tray Number:** - **Fixed Packing: Type:**								
Shape: - **Catalyst: Type:**	Fixed bed NiMo							
Shape: - -	Catalyst bed volume: 64 m^3							
Materials of Construction:	CS 2.25 Cr Internal: 3 mm SS 347	*Trays:* *Column*						
Other:		*Nr Trays: 28*						

Remarks:
1: Top stage/Condenser
2: Bottom stage/Reboiler

Equipment nr: **Name:**	(E01) Heat Exchanger	(E02) Heat Exchanger	*(E03)* *Heat Exchanger*	*(E07)* *Frac. Condenser*	*(E08)* *Cooler*	*(E09)* *Cooler*	*(E10)* *Cooler*
Substance **Tubes:**	Feed	Feed	*Feed*	*Light HC* H_2, H_2S, H_2O	*Gofinate*	*Distillate*	H_2, H_2S, H_2O, *C1-C5*
Shell:	H_2, H_2S, C1-C5 HC (light-medium boiling)	HC(medium-heavy boiling)	H_2, H_2S, *C1-C5 HC (light boiling)*	*n.a*	*n.a.*	*n.a.*	*n.a.*
Duty [kW]:	2043	3580	*4352*[1]	*-16056*	*-17914*	*-14400*	*-10900*
Heat exchange area [m²]:	169.7[4]	165.9[4]	*1870*[4]				
P [bar]: **Tubes:**	110	110	*110*	*3*	*3*	*3.8*	*100*
Shell:	3	3	*90*				
T [°C] **IN / OUT** **Tubes:**	250/288	288/308	*308/351*	*187/45*	*491/46*	*381/90*	*172/46*
Shell:	400/350	400/350	*400/318*				

Remarks: 1 Duties calculated with Aspen ®
2 Heat exchange areas based on method [16]
3. HC= Hydrocarbons
4. See … for calculation of heat exchange area's

Equipment nr: **Name:**	P01 Pump	*C01* *Compressor*
Medium transferred:	Heavy HC	*Treat-gas*
Capacity		
- **[l/hr]**	209394	*727190,17*
Density [kg/m³]	696	*24,8*
Pressure [bar]		
Suct. / Disch.:	90/110	*80/110*
Temperature **IN / OUT [°C]:**	389/390	*42.7/91.3*
Power [kW]		
- **Theoretically:**	31.4	
- **Actual:**	152,18	*1393,9*
Remarks:		

15.5 Equipment Specification Sheets

The following sheets contain information on equipment that is new, compared to the current installed Go-Finer. The fractionator is an exception.

Equipment Number: (D03)
Name: Fractionator

General Data

Service: Distillation
Column Type: tray
Tray Type: **cap / sieve / valve / ______**
Tray Number *(1)*
- **Theoretical:** 28
- **Actual:**
- **Feed (actual):** S127 STAGE 28
  S159 STAGE 28
  S143 STAGE 1
  S137 STAGE 8

Tray Distance (HETP) [m]: same as current
Tray Material : same as current
Column Diameter [m] : same as current
Colum Height [m] : same as current
Column Material : same as current
Pressure drop : 0.1 bar/ stage
Heating : open steam(actual) / reboiler (simulation)

Process Conditions

Stream Details	<S127>	<S137>	**Top <S138>**	**Bottom <S146A>**	**Reflux <S143>**	**Side stream <S161>**
Temp. [°C]	348	351	201	491	46	335
Pressure [bar]	5	3	3	5.7	3	3.8
Density [kg/m^3]	120	10.6	5,2	679	779	696
Mass Flow [kg/hr]	94357	39338	70354	60000	66053	76396

Component Split Fractions

	<S138>	<S146A>	<S161>
HYDROGEN	1,00	0,00	0,00
WATER	1,00	0,00	0,00
NH3	1,00	0,00	0,00
C3	1,00	0,00	0,00
C1	1,00	0,00	0,00
H2S	1,00	0,00	0,00
C2	1,00	0,00	0,00
IC4	1,00	0,00	0,00
NC4	1,00	0,00	0,00
NC5	1,00	0,00	0,00
CYCLOPEN	1,00	0,00	0,00
ISOHEX	1,00	0,00	0,00
NC6	1,00	0,00	0,00
PC185C	1,00	0,00	0,00
PC198C	1,00	0,00	0,00
PC212C	0,99	0,00	0,01
PC226C	0,93	0,00	0,07
PC240C	0,62	0,00	0,38
PC254C	0,19	0,00	0,81
PC267C	0,05	0,01	0,94
PC281C	0,02	0,01	0,97
PC295C	0,01	0,02	0,97
PC309C	0,00	0,03	0,97
PC323C	0,00	0,04	0,96
PC337C	0,00	0,05	0,95

PC350C	0,00	0,07	0,93
PC364C	0,00	0,09	0,91
PC378C	0,00	0,12	0,88
PC392C	0,00	0,16	0,84
PC406C	0,00	0,21	0,79
PC420C	0,00	0,27	0,73
PC439C	0,00	0,42	0,58
PC470C	0,00	0,94	0,06
PC495C	0,00	0,96	0,04
PC523C	0,00	0,98	0,02
PC549C	0,00	0,99	0,01
PC578C	0,00	0,99	0,01
PC607C	0,00	1,00	0,00
PC635C	0,00	1,00	0,00
PC664C	0,00	1,00	0,00

Column Internals

Same as current

Remarks: Tray numbering from top to bottom

Equipment Number: (E01)
Name: Heat exchanger

General Data

Type :Fixed Tube Sheets

Position:

Net Duty [kW]	: 2043	(Calculated)
Heat Exchange Area [m^2]	: 169.7	(Calculated)
Overall Heat Transfer Coefficient [$W/m^2 \cdot °K$]	: 113.6[1]	(Estimated)
LMTD(^0C)	: 106[2]	(Estimated)

Process Conditions

Medium TUBE side <Feed-S112>		**Medium Shell side <S126L>**	
Mass Stream [kg/hr]	: 140000	**Mass Stream[kg/hr]**	: 37503,26
Average Specific Heat[kJ/kg]	: -1039,51	**Average Specific Heat [kJ/kg]**	: -412,13
Temperature IN [°C]	: 250	**Temperature IN [°C]**	: 400
Temperature OUT [°C]	: 287	**Temperature OUT [°C]**	: 350
Pressure [bar]	: 110	**Pressure [bar]**	: 3
Material	: Heavy Feed	**Material**	: Light Hydrocarbons, H_2, H_2O

Remarks: 1: From [13]
2: See… for calculations

Equipment Number: (E02)
Name: Heat exchanger

General Data

Type :Fixed Tube Sheets

Position:

Net Duty [kW] : 3520 (Calculated)
Heat Exchange Area [m^2] : 165.9 (Calculated)
Overall Heat Transfer Coefficient [$W/m^2\cdot°K$]: 284[1] (Estimated)
LMTD(^{0}C) : 76[2] (Estimated)

Process Conditions

Medium TUBE side <S113>
Mass Stream [kg/hr] : 140000
Average Specific Heat[kJ/kg] : -986,97
Temperature IN [°C] : 287
Temperature OUT [°C] : 308
Pressure [bar] : 110
Material : Heavy Feed

Medium Shell side <S126L>
Mass Stream[kg/hr] : 93357
Average Specific Heat [kJ/kg] : -708,26
Temperature IN [°C] : 400
Temperature OUT [°C] : 350
Pressure [bar] : 3
Material : Medium-Heavy boiling HC, H_2, H_2O

Remarks: 1: From [13]
2: See 15-83 for calculations

Equipment Number: (E03)
Name: Heat exchanger

General Data

Type :Fixed Tube Sheets

Position:

Net Duty [kW] : 3520 (Calculated)
Heat Exchange Area [m^2] : 1870 (Calculated)
Overall Heat Transfer Coefficient [$W/m^2\cdot°K$]: 113.6[1] (Estimated)
LMTD(^{0}C) : 25[2] (Estimated)

Process Conditions

Medium TUBE side <S114>
Mass Stream [kg/hr] : 140000
Average Specific Heat[kJ/kg] : -894,92
Temperature IN [°C] : 308
Temperature OUT [°C] : 359
Pressure [bar] : 110
Material : Heavy Feed

Medium Shell side <S116V>
Mass Stream[kg/hr] : 44673
Average Specific Heat [kJ/kg] : -334,8
Temperature IN [°C] : 400
Temperature OUT [°C] : 318
Pressure [bar] : 90
Material : *H_2, H_2S, C1-C5, HC(light boiling)*

Remarks: 1: From [13]
2: See 15-83 for calculations

Equipment Number: C01
Name : Treat-gas recycle compressor
Operating : 1
Installed Spare: 0

Service : Treat-gas compressor
Type : Isentropic Centrifugal Compressor
Number: 1

Operating Conditions & Physical Data

Compressed Gasses : H_2, Light Hydrocarbons
Temperature Inlet ***(T)*** **[°C]** : 42.7
Calculated Outlet Temperature[°C] : 91.3
Density ***(ρ)*** **[kg/m^3]** : 24,8
Vapour fraction : 0.9

Power

Capacity (Φ_v) [m^3/s] : 2.02
Suction Pressure (p_s) [bar] : 80
Discharge Pressure (p_d) [bar] : 110

Net Work required [kW] : 1393,9
Isentropic Efficiency [-] : 0.72
Mechanical Efficiency [-] : 1.00
Power at Shaft [kW] :

Construction Details

Same as current	

Construction Materials

Same as current	

Remarks:

Equipment Number: P01
Name: Reactor (R03) liquid feed pump
Operating : 1
Installed Spare: 0

Service : Feed pump
Type : Centrifugal

Operating Conditions & Physical Data

Pumped Liquid: Heavy Hydrocarbons
Temperature ***(T)*** **[°C]:** 388
Density ***(ρ)*** **[kg/m^3]:** 696

Power

Capacity (Φ_v) [m^3/s] :209.4
Suction Pressure (p_s) [bar] : 90
Discharge Pressure (p_d) [bar] :110
Theoretical Power [kW] : 418000 **{$= \Phi_v (p_d-p_s)10^2$}**
Pump Efficiency [-] : 0.76

Construction Details[1]

RPM : 3000	- **N.P.S.H. [m]** : 0,66 **{$=p_m \rho g$}**
Drive : Electrical	
Tension [V] : 380	
Rotational direction : Clock	
Foundation plate : Combined	
Flexible Coupling : Yes	
Pressure Gauge Suction : No	
Pressure Gauge Discharge : Yes	
Min. Overpressure Above p_v/p_m [bar]: n.a.	

Construction Materials[1]

Pump House : MS	**Wear Rings:**
Pump Rotor : Steel	**Shaft Box:**
Shaft : Steel	
Special provisions:	
Operating pressure [bar] : 90-110	**Test Pressure [bara]:**

Remarks: 1. From [17]

The heat exchange area can be determined using the following equations:

φ_q=U.A.LMTD

$$\text{LMTD}=\frac{(T_1-t_2)-(T_2-t_1)}{\ln\left(\frac{T_1-t_2}{T_2-t_1}\right)}$$

φ_q =Heat duty obtained from Aspen

T= temperature material that will be cooled
t= temperature of medium that will be heated

U= Overall heat transfer coefficient and can be estimated from literature [13]

15.6 Economy

15.6.1 Investment Cost

15.6.1.1 “Lang-factors”

“Lang-Factors” for investment costs are divided in factors for direct costs and indirect costs. In the normal case where only new units are built, the “Lang-factors” will be the same for all units. In this case however, new units are built and ‘old’-units are adapted for the new design with minor or major changes. Therefore in this case, the “Lang-factors” for each unit are determined separately.

Table 15.12: Important “Lang-factors” for each new and changed unit [16]

“ Lang-Factor”		Value					
			(R03)	(R02)	(E01)	(E02)	(P01)
Direct costs							
f1	Equipment erection	0.40	0.40	0.40	0.40	0.40	0.40
f2	Piping	0.70	0.70	0.70	0.70	0.70	0.70
f3	Instrumentation	0.20	0.20	-	0.20	0.20	0.20
f4	Electrical	0.10	0.10	-	0.10	0.10	0.10
f5	Buildings, process	0.15	0.15	-	0.15	0.15	0.15
f6	Utilities	0.50	-	-	-	-	-
f7	Storages	0.15	-	-	-	-	-
f8	Site development	0.05	-	-	-	-	-
f9	Ancillary building	0.15	-	-	-	-	-
Total Direct		**3.40**	**2.55**	**1.10**	**2.55**	**2.55**	**2.55**
Indirect costs							
f10	Design and Engineering	0.30	0.30	0.30	0.30	0.30	0.30
f11	Contractor’s fee	0.05	0.05	0.05	0.05	0.05	0.05
f12	Contingency	0.10	0.10	0.10	0.10	0.10	0.10
Total Indirect		**1.45**	**1.45**	**1.45**	**1.45**	**1.45**	**1.45**

Remarks:

- The total direct and total indirect “Lang-factors” are summedm and in the direct “Lang-factor” a factor 1 is added (except for (R02)).
- f6, f7, f8 and f9 are not added for the new and changed units, because those factors are only important for building an entirely new plant.
- For the cost estimation of the changes in (R02), only f1 and f2 are taken into account (together with all the factors for indirect costs). As the additional “Langdirect factor” of 1 represents the costs for manufacturing a new vessel, this factor is now not taken into account. The cost for the remodelling will be in equipment erection (structural work) and piping (including insulation and painting of new parts in the unit) as represented in the “Lang factors” f1 and f2.

15.6.1.2 Reactor 3 (R03)

For the calculation of the purchase cost of (R03), the following data is known and required for calculations:

Table 15.13: RequiredR parameters for calculation of purchase cost of (R03).

Reactor Vessel 3 (R03)	
Type	Vertical Vessel
Volume (m^3)	70.4
Diameter (m)	3.0
Height (m)	10.0
Pressure (bar)	110

Material of construction	Stainless Steel

Assumptions:

- Volume of reactor vessel is $1.10*V_{cat,(R03)}$
- For cost estimation, chosen diameter for reaction vessel is 3.0m

Purchase cost = equipment cost * pressure factor * material factor
Equipment costs are adapted from [16]

Equipment cost: 40k$
Material factor: 2.0 (stainless steel)

It is known that regularly the reactor will be constructed with a carbon steel outside and a stainless steel corrosion protective layer. However, no data was found how to combine this in the current calculation method. Therefore, a stainless steel reactor is assumed. An additional advantage of this approach is that an extra safety margin is now accounted for.

The pressure in (R03) is beyond the given pressure factors. Therefore the pressure factors are extrapolated to get an estimation of the pressure factor at p=110bar. The correlation is given in Figure 15.1.

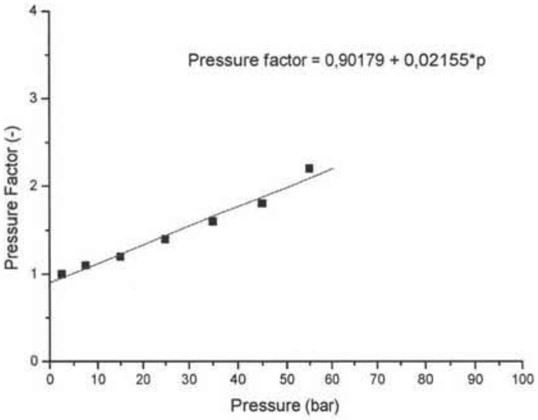


Figure 15.1: Correlation between pressure factor and pressure in reactor vessels.

The data has been fit with a linear relation, which results in a pressure factor of 3.27 at p=100bar.
This makes the purchase cost of (R03): Ce = 261.6k$

15.6.1.3 Reactor 2 (R02)

For the calculation of the cost for (R02), the following data is known and required for calculations:

Table 15.14: Required parameters for calculation of purchased cost of (R02).

Reactor Vessel 2 (R02)	
Type	Vertical Vessel
Volume (m^3)	119.35
Diameter (m)	3.0
Height (m)	16.9
Pressure (bar)	90
Material of construction	Stainless Steel

The same assumptions and equations are used as in the previous paragraph
Equipment cost: 70k$
Material factor: 2.0 (stainless steel)
Pressure factor: 2.84 (see 15-83)
This makes the purchased cost of (R02): Ce = 397.6k$

15.6.1.4 Heat-Exchanger 1 (E01)

For the calculation of the purchase cost of (E01), the following data is known and required for calculations:

Table 15.15: Required parameters for calculation of purchased cost of (E01).

Heat Exchanger 1	
Material Shell	Stainless Steel
Material Tube	Stainless Steel
Pressure (bar)	110
Type	Fixed Tube Sheet
Heat Transfer Area (m^2)	169.7

Purchase cost = equipment cost * pressure factor * type factor
Equipment costs are adapted from [16]
Equipment cost: 80k$
Type factor: 0.8 (fixed tube sheet)

The pressure in (E03) is beyond the given pressure factors. Therefore the pressure factors are extrapolated to get an estimation of the pressure factor at p=110bar. The correlation is given in Figure 15.2.

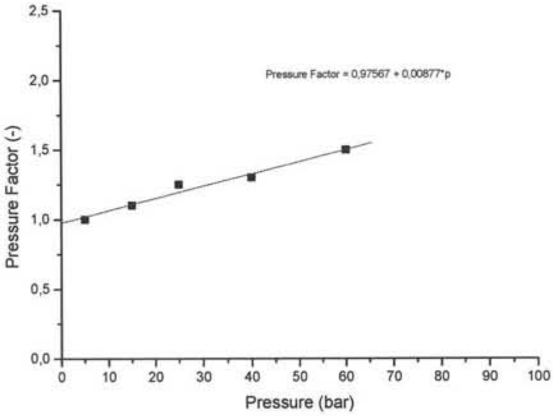


Figure 15.2: Correlation between pressure factor and pressure in heat exchangers.

The data has been fit with a linear relation, which results in a pressure factor of 1.94 at p=110bar. This makes the purchase cost of (E03): Ce = 124.2k$

15.6.1.5 Heat Exchanger 2 (E02)

For the calculation of the purchased cost of (E02), the following data is known and required for calculations:

Table 15.16: Required parameters for calculation of purchased cost of (E02).

Heat Exchanger 2	
Material Shell	Stainless Steel
Material Tube	Stainless Steel
Pressure (bar)	110
Type	Fixed Tube Sheet
Heat Transfer Area (m^2)	165.9

Equipment cost: 80k$
Type factor: 0.8 (fixed tube sheet)
Pressure Factor: 1.94
This makes the purchased cost of (E04): Ce = 124.2k$

15.6.1.6 Pump 1 (P01)

For determination of the investment cost for specific units, the following formula is given:
$Ce = C * S^n$ [16]
Ce is the purchased equipment cost, S the characteristic size parameter, C the cost constant and n the index for specific type of equipment.
For (P01), these are given in Table 15.17.

Table 15.17: Parameters for determination of the purchase costs for (P01)

Pump 1 (P01)	
S (-)	152
C ($)	960 [16]
n (-)	0.8 [16]

This makes the purchase equipment costs of (P01): Ce = 53.4k$

15.6.2 Operating Costs

15.6.2.1 Raw Materials

Raw materials for the new design will be H_2 and Catalyst (it is chosen to calculate the catalyst used as an operating cost instead of an investment cost, because after each period of 1.5yr, catalyst beds need to be changed). In Table 15.18 the calculation of the materials costs can be found.

Table 15.18: Raw material costs (as deviations from current process)

Raw Material	Amount (t/h)	Costs raw material ($/t)	Costs per hour ($/h)	Costs per year (k$/yr)
Catalyst (R01)	n.a.	n.a.	n.a.	n.a.
Catalyst (R02)	n.a.	n.a.	n.a.	n.a.
Catalyst (R03)	0.0034	19.9	68	585
Feed	n.a.	n.a.	n.a.	n.a.
Hydrogen	6.08	1500	9120	78487
Total			**9188**	**79072**

Remarks:

- Catalyst required per hour :
  - Density catalyst bed: 700kg/m^3
  - Volume catalyst bed (R03): 64m^3
  - Price catalyst (NiMo): 20$/kg (19.9k$/t)

  - Catalyst replacement in 1.5 year; offline during 10 days.
  - (R03) online per year: 8606 h/yr (needed for calculation to costs per year)
  - Amount Catalyst (t/h) = (64*700/1000)*1/1.5*(365*24) = 0.0034
- Hydrogen required per hour:
  - Current hydrogen usage per hour: 1.8t/h
  - 'New" hydrogen usage per hour: 7.88t/h
  - Extra hydrogen usage per hour: 6.08t/h

15.6.2.2 Utilities

Utilities required in the new design of the GO-finer can be found in 5.3. The costs of utilities are given by the project principles. With the use of Table 15.19, the costs for utilities are determined.

Table 15.19: Utility costs of the new designed equipment. (Utilities required for existing equipment and units is assumed to be constant)

Utility	Utility Price (\$/t for 1-5) (\$/MWhf for 6) (\$/MWhe for 7)	Utility Required (t/hr for 1-5) (MWhf for 6) (MWhe for 7)	Utility Costs (\$/hr)	Utility Costs (k\$/yr)
(1) Steam-1	5.3	0	0	0
(2) Steam-3	5.3	0	0	0
(3) Steam-9	7.3	0	0	0
(4) Steam-40	10.2	0	0	0
(5) Cooling Water	0.8	0	0	0
(6) Heating Oil	12.0	0	0	0
(7) Electricity	70.5	0.152	10.7	93.4
Total			**10.7**	**93.4**

15.7 Matlab

15.7.1 Matlab ® scripts

For the determination of the kinetic parameters the following Matlab ® scripts were used:

- self.m
- RX2_fun_tot.m
- dfdV_all.m
- reac.m
- stoich.m

The script self.m should be run to calculate and get answers. It uses RX2_fun_tot.m and loads export.mat, which contains several factors with component distributions, molecular weight of the components and the sulphur and nitrogen content of the components. RX2_fun_tot calculates the molar flow profile of the components in the reactor along the reactor volume. It uses the script dfdV.m, which gives the differential equations of all the component mass balances (mole based), and calls upon reac.m and stoich.m. The script reac.m contains the reaction rates and stoich.m the stoichiometric matrix for all reactions.
After self.m has run, it will save the results in a file import.mat, it creates a figure with the hydrogen molar flow profile and it saves the exit molar flows of all components in tuning.txt.

For the determination of the volume of the new reactor (RX2) the following Matlab ® scripts were used:

- run_RX2_RX3.m

- RX2_fun_tot.m
- RX3_fun.m
- dfdV_all.m
- reac.m
- stoich.m

The script run_RX2_RX3.m should be run to calculate and get answers. It uses RX2_fun_tot.m for the calculations of RX2 and RX3_fun.m for the calculations of RX3. It loads import.mat created by self.m. Both RX2_fun_tot.m and RX3_fun.m calculate the molar flow profile in the reactors (RX2_fun_tot.m for RX2 and RX3_fun.m for RX3) and use dfdV.m, which give the differential equations. The scripts reac.m and stoich.m are again used by dfdV.m to obtain the reaction rates and the stoichiometric matrix.

After run_RX2_RX3.m has run, it will save the results in results.mat, it will create two subplots in one figure with the hydrogen molar flow profiles in RX2 and RX3 and it will save the molar flow profiles of all components in results2.txt and results3.txt.

15.7.2 Matlab ® model equations

The model used to calculate the molar flow profile in the reactor system. The kinetic model used for the calculations is given by eq. 8.1.

$$R_i = \frac{k_i \cdot \phi_j \cdot \phi_{H_2}}{1 + K \cdot C_{H_2S}} \qquad \text{(eq. 8.1)}$$

$$R_i = \frac{k_i' \cdot C_j \cdot C_{H_2}}{1 + K \cdot C_{H_2S}} = \frac{\frac{k_i'}{\phi_V^{\,2}} \cdot \phi_V \cdot C_j \cdot \phi_V \cdot C_{H_2}}{1 + K \cdot C_{H_2S}} = \frac{k_i \cdot \phi_j \cdot \phi_{H_2}}{1 + K \cdot C_{H_2S}} \qquad \text{(eq.8.1a)}$$

R_i is reaction rate of reaction i

k_i is the kinetic parameter of reaction i

ϕ_j is the molar flow of component j, reactant in reaction i

ϕ_{H_2} is the molar flow of H_2

K is the adsorption constant for H_2S

C_{H_2S} is the concentration of H_2S

C_{H_2} is the concentration of H_2

C_i is the concentration of component j, reactant in reaction i

ϕ_V is the volumetric flow rate

k_i' is the kinetic parameter of reaction i based on concentrations

$$R = \begin{bmatrix} R_1 \\ R_2 \\ \vdots \\ R_{nr} \end{bmatrix} \qquad \text{(eq. 8.2)}$$

nr is number of reactions

The stoichiometric matrix for all components and all reactions is given by eq. 8.3.

$$\nu=\begin{bmatrix}\nu_{1,1} & \nu_{1,2} & \cdots & \nu_{1,nc}\\ \nu_{2,1} & \nu_{2,2} & \cdots & \nu_{2,nc}\\ \vdots & \vdots & & \vdots\\ \nu_{nr,1} & \nu_{nr,2} & \cdots & \nu_{nr,nc}\end{bmatrix} \qquad \text{(eq. 8.3)}$$

nc is number of components

$\nu_{i,j}$ is stoichiometric coefficient of component j in reaction i

The net rate of production of all components based on all reactions is given by eq. 8.4.

$$r=\begin{bmatrix}r_1\\ r_2\\ \vdots\\ r_{nc}\end{bmatrix}=\begin{bmatrix}\nu_{1,1}\cdot R_1 & \nu_{2,1}\cdot R_2 & \cdots & \nu_{nr,1}\cdot R_{nr}\\ \nu_{1,2}\cdot R_1 & \nu_{2,2}\cdot R_2 & \cdots & \nu_{nr,2}\cdot R_{nr}\\ \vdots & \vdots & & \vdots\\ \nu_{1,nc}\cdot R_1 & \nu_{2,nc}\cdot R_2 & \cdots & \nu_{nr,nc}\cdot R_{nr,nc}\end{bmatrix}=\nu^T\cdot R \qquad \text{(eq. 8.4)}$$

r_i is the net rate of production of component i

The molar balance for component i and all reactions is given by eq. 8.5.

$$0=\phi_i\big|_V-\phi_i\big|_{V+\Delta V}+r_i\cdot\Delta V \Leftrightarrow \frac{d\phi_i}{dV}=r_i \qquad \text{(eq. 8.5)}$$

V is the catalyst bed volume

The total molar balance for all components and all reactions is given by eq. 8.6.

$$\frac{d\phi}{dV}=r=\nu^T\cdot R \qquad \text{(eq. 8.6)}$$

Equation 6 gives a vector with as many rows as there are components, if this differential equation is solved over the volume of the catalyst bed it will give the molar flow profile of all components present in the reactor.

15.7.3 Model equations BoD

The model equations for preliminary calculations used for the BoD are given below. From the literature it is known that a lumped model as given by eq. 7 can be used to describe a system with several organic sulfur containing components.

$$r=\frac{k\cdot C_{org-S}{}^{2}\cdot C_{H_2}}{1+K\cdot C_{H_2S}} \qquad \text{(eq. 8.7)}$$

r is reaction rate

k is the kinetic parameter of the reaction

C_{org-S} is the concentration of the organic sulfur containing components

C_{H_2} is the concentration of H_2

K is the adsorption constant for H_2S

C_{H_2S} is the concentration of H_2S

The molar balance for an ideal plug flow reactor is given by eq. 8.8.

$$0 = \left(C_{org-S}\Big|_{V} - C_{org-S}\Big|_{V+\Delta V} \right) \cdot \phi_V + r \cdot \Delta V \Leftrightarrow \frac{dC_{org-S}}{dV} = \frac{r}{\phi_V} \qquad \text{(eq. 8.8)}$$

ϕ_V is the volumetric flow rate

V is the catalyst bed volume

In eq. 8.9 the conversion X is introduced.

$$X = \frac{\left(C_{org-S0} - C_{org-S} \right)}{C_{org-S0}}$$

$$C_{org-S} = C_{org-S0} \cdot (1 - X) \qquad \text{(eq. 8.9)}$$

$$C_{H_2S} = C_{org-S0} \cdot X$$

X is the conversion of organic sulfur containing components

C_{org-S0} is the concentration of organic sulfur containing components at reactor inlet

Combining eq. 8.7 to 8.9 gives eq. 8.10. Eq. 8.10 can be rewritten as differential equation (eq. 8.11), which can be solved analytically. It is assumed that the hydrogen concentration is constant within the reactor. The analytical solution written to solve k based on the known conversion is given by eq. 8.12 and the analytical solution to solve a reactor volume based on a known k and conversion is given by eq. 8.13.

$$\phi_V \cdot C_{org-S0} \cdot \frac{dX}{dV} = \frac{k \cdot C_{org-S0}{}^2 \cdot (1-X)^2 \cdot C_{H_2}}{1 + K \cdot C_{org-S0} \cdot X} \qquad \text{(eq. 8.10)}$$

$$\frac{k \cdot C_{org-S0}{}^2 \cdot V \cdot C_{H_2}}{\phi_V \cdot C_{org-S0}} = \int_0^X \frac{\left(1 + K \cdot C_{org-S0} \cdot X\right)}{(1-X)^2} dX \qquad \text{(eq. 8.11)}$$

$$k = \frac{\phi_V \cdot C_{org-S0}}{C_{org-S0}{}^2 \cdot V \cdot C_{H_2}} \cdot \left[\frac{\left(1 + K \cdot C_{org-S0}\right) \cdot X}{(1-X)} - K \cdot C_{org-S0} \cdot \ln\left(\frac{1}{1-X}\right) \right] \qquad \text{(eq. 8.12)}$$

$$V = \frac{\phi_V \cdot C_{org-S0}}{C_{org-S0}{}^2 \cdot k \cdot C_{H_2}} \cdot \left[\frac{\left(1 + K \cdot C_{org-S0}\right) \cdot X}{(1-X)} - K \cdot C_{org-S0} \cdot \ln\left(\frac{1}{1-X}\right) \right] \qquad \text{(eq. 8.13)}$$

15.7.4 Matlab ® results

In Table 15.20 the kinetic parameters and the mass flow profile of the components leaving (R02) and (R03) are given. The volumes of the two catalyst beds are 108.5 m^3 and 64 m^3 respectively; the results given in chapter 0 are based on the mass flows in Table 15.20.
Component ID is based on the provided component distribution [7]. The first number gives the column starting at the left, the second number gives the component starting at the top and the letter gives the row. The saturates have one row labelled with the 'f', the aromatics have five rows labelled 'a' to 'e', the sulphides have one row labelled 'g' and the polars have two rows labelled 'h' and 'i'. Because in row 'h' no component is present after the reactions have taken place in the current reactor and because the components of this row are present in the feed for 0.53 wt%, it was chosen to neglect this row.

15.7.5 Matlab ® scripts

Columns have been added to make documentation more compact.

- Self.m:

```
% The file self.m calculates the kinetic parameters based on the
% conversions of components. It loads export.mat andd uses RX2fun.m
% RX3fun.m. These file use dfdV_all.m and stoich.m and reac.m will be used
% by dfdV_all.m.

clear all
format compact
format short e

global  z  rho  phi_m_in  phi_m_end  K  Mwt  wt_per_in  wt_per_end  phi_end
h2_quench n

load export.mat

z = 0.5;                % [-] liquid fraction of the feed
rho = 730;                 % [kg/m^3] density of the liquid fraction of the
feed
phi_m_in = 136e3;       % [kg/h] mass stream of the HC feed
phi_m_end = 127.8e3;    % [kg/h] mass stream of the HC effluent
K = 2.34;               % [m^3/mol]

% Molecular weight of the components
Mwt = [0.034;
    0.017;
    0.002;
    0.035;
    Mwt];

% The inlet composition
wt_per_in = feed;

% The exit composition
wt_per_end = Product;

% Mass flows leaving the reactor
% H2S, NH3, H2, light gas
mass_gas_in = [0;0;5600;0];

% Mass flows leaving the reactor
% H2S, NH3, H2, light gas
mass_gas_end = [6300;680;6900;3000];

% The molar flows at exit of reactor
phi_end = [mass_gas_end;phi_m_end/100*wt_per_end]./Mwt

h2_quench = 3100/(0.002*4); % [mol/h], total quench is about 3.1 [ton/h]

% Number of rate constants that need to be estimated
n = 138;

%  Estimate  of  rate          0.073;                        0.35;
constants                      0.05;                         0.218;
k = [0.2;                      0.05;                         0.055;
    0.073;                     0.35;                         0.155; %10
```

```
    0.24;
    0.118;
    0.05;
    0.05;
    0.475;
    0.081;
    0.077;
    0.078;
    0.27;
    0.27; %20
    0.009;
    0.8;
    0.009;
    0.395;
    0.086;
    0.074;
    0.091;
    0.108;
    3.04;
    0.205;    %30
    0.0012;
    0.0415;
    0.05;
    0;
    0.27;
    0.17;
    0.31;
    0.031;
    0.01;
    0.22; %40
    3.8;
    0.434;
    0.23;
    0.475;
    0.01;
    0.205;
    0.52;
    0.27;
    5.1;
    0.080; %50
    0.431;
    4.95;
    0.157;
    2.8;
    3.0;
    0.201;
    0.204;
    0.204;
    0.72;
    4.51; %60
    8.27;
    0.086;
    2.53;
    2.68;
    0.157;
    0.595;
    7.56;
    5.36;
    0.201;
    0.206; %70
    0.206;
    0.319;
    0.154;
    0.154;
    14.7;
    5.76;
    11.47;
    0.21;
    0.205;
    0.41; %80
    0.683;
    0.428;
    0.195;
    0.21;
    0.0012;
    0.201;
    0.4320;
    0.001;
    0.0015;
    0.0001; %90
    0.0001;
    0.1;
    0.184;
    0.415;
    4.46;
    8.16;
    2.23;
    7.2;
    4.1;
    8.65; %100
    4.17;
    7.47;
    15.1;
    0.086;
    0.35;
    0.21;
    0.208;
    0.217;
    0.22;
    0.74; %110
    0.95;
    0.205;
    0.215;
    0.388;
    0.305;
    0.38;
    0.1;
    0.108;
    0.23;
    0.597; %120
    425e3;
    72.5e3;
    0.108;
    0;
    0.205;
    0;
    0.202;
    0;
    0.405;
    0.077; %130
    0.195;
    0.58;
    0.621;
    0.0415;
    0.3;
    0.225;
    0.17;
    0.089];

% Save the results as parameter vector
param(1:n) = k(1:n);

% Inlet molar streams
phi0 = ([mass_gas_in;phi_m_in/100*wt_per_in]./Mwt);

% Calculate the molar flows for the catalyst bed volume
[RX2,m1,m2] = RX2fun_tot(phi0,param);

% Saving the results in a txt file:
file = fopen('tuning.txt', 'w');
phi_calc = RX2(m1,2:m2)';
SSres = (phi_end - phi_calc)./phi_end).^2;
error = ones(1,length(SSres)*SSres
for i = 1:m2-1
    fprintf(file, '%15.7f  %15.9f\n', phi_calc(i,1), SSres(i,1);
end
```

```
fclose(file);

% Sulphur content:
S_factor = Mwt(5:(m2-1),1).*Scontent;
S_mass = RX2(m1,6:m2)*S_factor
S_wt_per = S_mass*100/phi_m_end

% Nitrogen content:
N_factor = Mwt(5:(m2-1),1).*Ncontent;
N_mass = RX2(m1,6:m2)*N_factor
N_wt_per = N_mass*100/phi_m_end

% Save results in a workspace
savefile = 'import.mat';
save(savefile, '-mat');



figure(2)
plot(RX2(:,1),RX2(:,4))
title('Molar flow profile in RX2')
xlabel('Volume of catalyst bed /[m^3]')
ylabel('Molar flows of H2 /[mol/h]')
```

- RX2fun.m:

```
function [RX2,m1,m2] = RX2fun(phi0,param)

global  z  rho  phi_m_in  phi_m_end  K  Mwt  wt_per_in  wt_per_end  phi_end
h2_quench n

% Options for the integration
options = odeset('AbsTol', 1e-3, 'RelTol', 1e-3);

% Boundary conditions and domain
V0 = 0;                    % [m^3] initial volume
V1 = 12.5;                 % [m^3] volume of first catalyst bed
V2 = 12.5 + 32;            % [m^3] volume of second catalyst bed
V3 = 12.5 + 2 * 32;        % [m^3] volume of third catalyst bed
Vf = 12.5 + 3 * 32;        % [m^3] volume of fourth catalyst bed

% First integration
Vspan = [V0 V1];           % integration domain
phi0(1,3) = phi0(1,3) + h2_quench;
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);

% Second integration
Vspan = [V1 V2];           % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench;
phi0 = phi(length(V),:);
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);

% Third integration
Vspan = [V2 V3];           % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench;
phi0 = phi(length(V),:);
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);

% Fourth integration
Vspan = [V3 Vf];           % integration domain
```

```
phi(length(V),3) = phi(length(V),3) + h2_quench;
phi0 = phi(length(V),:);
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);

bed4 = [V phi];
% Size of the matrix
[m1,m2] = size(bed4);

% Save results in one vector
RX2 = bed4(m1,:);
```

- dfdV_all.m:

```
function dfdV = dfdV_all(V,phi,flag,param)

global  z  rho  phi_m_in  phi_m_end  K  Mwt  wt_per_in  wt_per_end  phi_end  h2_quench n

% The rate constants
 k = param;

% Easy notation
h2s = phi(1);

% All reaction rates per reaction
R = reac(phi,k);

% Stoichiometric coefficient matrix
nu = stoich(R);

% The model equations:
dfdV = nu'*R/(1+K*z*phi_m_in/rho*h2s);
```

- reac.m:

```
function R = reac(phi, k)

% Easy notation
h2 = phi(3);

R(1:41,1) = [k(1)*h2*phi(100);
    k(2)*h2*phi(91);
    k(3)*h2*phi(91);
    k(4)*h2*phi(82);
    k(5)*h2*phi(82);
    k(6)*h2*phi(63);
    k(7)*h2*phi(63);
    k(8)*h2*phi(71);
    k(9)*h2*phi(59);
    k(10)*h2*phi(114);
    k(11)*h2*phi(122);
    k(12)*h2*phi(89);
    k(13)*h2*phi(80);
    k(14)*h2*phi(80);
    k(15)*h2*phi(70);
    k(16)*h2*phi(56);
    k(17)*h2*phi(105);
    k(18)*h2*phi(103);
    k(19)*h2*phi(92);
    k(20)*h2*phi(92);
    k(21)*h2*phi(85);
    k(22)*h2*phi(65);
    k(23)*h2*phi(85);
    k(24)*h2*phi(54);
    k(25)*h2*phi(61);
    k(26)*h2*phi(86);
    k(27)*h2*phi(53);
    k(28)*h2*phi(57);
    k(29)*h2*phi(62);
    k(30)*h2*phi(116);
    k(31)*h2*phi(87);
    k(32)*h2*phi(76);
    k(33)*h2*phi(79);
    k(34)*h2*phi(72);
    k(35)*h2*phi(78);
    k(36)*h2*phi(81);
    k(37)*h2*phi(55);
    k(38)*h2*phi(84);
    k(39)*h2*phi(58);
    k(40)*h2*phi(60);
```

```
    k(41)*h2*phi(64)];

R(42:46,1) = [k(42)*h2*phi(66);
    k(43)*h2*phi(94);
    k(44)*h2*phi(69);
    k(45)*h2*phi(83);
    k(46)*h2*phi(116)];

R(47:77,1) = [k(47)*h2*phi(67);
    k(48)*h2*phi(77);
    k(49)*h2*phi(26);
    k(50)*h2*phi(75);
    k(51)*h2*phi(99);
    k(52)*h2*phi(23);
    k(53)*h2*phi(109);
    k(54)*h2*phi(97);
    k(55)*h2*phi(21);
    k(56)*h2*phi(101);
    k(57)*h2*phi(106);
    k(58)*h2*phi(106);
    k(59)*h2*phi(95);
    k(60)*h2*phi(32);
    k(61)*h2*phi(19);
    k(62)*h2*phi(121);
    k(63)*h2*phi(18);
    k(64)*h2*phi(27);
    k(65)*h2*phi(111);
    k(66)*h2*phi(118);
    k(67)*h2*phi(37);
    k(68)*h2*phi(25);
    k(69)*h2*phi(102);
    k(70)*h2*phi(108);
    k(71)*h2*phi(108);
    k(72)*h2*phi(115);
    k(73)*h2*phi(112);
    k(74)*h2*phi(112);
    k(75)*h2*phi(34);
    k(76)*h2*phi(38);
    k(77)*h2*phi(22)];

R(78:84,1) = [k(78)*h2*phi(127);
    k(79)*h2*phi(132);
    k(80)*h2*phi(126);
    k(81)*h2*phi(50);
    k(82)*h2*phi(52);
    k(83)*h2*phi(43);
    k(84)*h2*phi(39)];

R(85:94,1) = [k(85)*h2*phi(87);
    k(86)*h2*phi(107);
    k(87)*h2*phi(7);
    k(88)*h2*phi(9);
    k(89)*h2*phi(11);
    k(90)*h2*phi(78);
    k(91)*h2*phi(84);
    k(92)*h2*phi(51);
    k(93)*h2*phi(47);
    k(94)*h2*phi(68)];

R(95:117,1) = [k(95)*h2*phi(17);
    k(96)*h2*phi(35);
    k(97)*h2*phi(24);
    k(98)*h2*phi(31);
    k(99)*h2*phi(29);
    k(100)*h2*phi(28);
    k(101)*h2*phi(36);
    k(102)*h2*phi(33);
    k(103)*h2*phi(30);
    k(104)*h2*phi(123);
    k(105)*h2*phi(20);
    k(106)*h2*phi(40);
    k(107)*h2*phi(49);
    k(108)*h2*phi(130);
    k(109)*h2*phi(125);
    k(110)*h2*phi(129);
    k(111)*h2*phi(128);
    k(112)*h2*phi(131);
    k(113)*h2*phi(124);
    k(114)*h2*phi(41);
    k(115)*h2*phi(46);
    k(116)*h2*phi(44);
    k(117)*h2*phi(51)];

R(118:138,1) = [k(118)*h2*phi(93);
    k(119)*h2*phi(96);
    k(120)*h2*phi(98)
    k(121)*phi(14);
    k(122)*phi(15);
    k(123)*h2*phi(6);
    k(124)*h2*phi(7);
    k(125)*h2*phi(8);
    k(126)*h2*phi(9);
    k(127)*h2*phi(10);
    k(128)*h2*phi(11);
    k(129)*h2*phi(41);
    k(130)*h2*phi(90);
    k(131)*h2*phi(45);
    k(132)*h2*phi(48);
    k(133)*h2*phi(74);
    k(134)*h2*phi(76);
    k(135)*h2*phi(113);
    k(136)*h2*phi(119);
    k(137)*h2*phi(104);
    k(138)*h2*phi(88)];
```

- stoich.m:

```
function nu = stoich(R)

% Create empty stoichiometric matrix
nu = sparse(zeros(length(R),132);
```

```
% HYD reactions of aromatic rings (k(1) till k(41)
nu(1,3) = -2; nu(1,100) = -1; nu(1,91) = 1;
nu(2,3) = -2; nu(2,91) = -1; nu(2,82) = 1;
nu(3,3) = -1; nu(3,91) = -1; nu(3,63) = 1;
nu(4,3) = -2; nu(4,82) = -1; nu(4,71) = 1;
nu(5,3) = -4; nu(5,82) = -1; nu(5,59) = 1;
nu(6,3) = -3; nu(6,63) = -1; nu(6,71) = 1;
nu(7,3) = -5; nu(7,63) = -1; nu(7,59) = 1;
nu(8,3) = -2; nu(8,71) = -1; nu(8,6) = 1;
nu(9,3) = -2; nu(9,59) = -1; nu(9,6) = 1;
nu(10,3) = -2; nu(10,114) = -1; nu(10,122) = 1;
nu(11,3) = -2; nu(11,122) = -1; nu(11,89) = 1;
nu(12,3) = -2; nu(12,89) = -1; nu(12,80) = 1;
nu(13,3) = -2; nu(13,80) = -1; nu(13,70) = 1;
nu(14,3) = -4; nu(14,80) = -1; nu(14,56) = 1;
nu(15,3) = -3; nu(15,70) = -1; nu(15,5) = 1;
nu(16,3) = -1; nu(16,56) = -1; nu(16,5) = 1;
nu(17,3) = -13; nu(17,105) = -1; nu(17,73) = 1;
nu(18,3) = -2; nu(18,103) = -1; nu(18,90) = 1;
nu(19,3) = -2; nu(19,92) = -1; nu(19,85) = 1;
nu(20,3) = -1; nu(20,92) = -1; nu(20,65) = 1;
nu(21,3) = -2; nu(21,85) = -1; nu(21,54) = 1;
nu(22,3) = -3; nu(22,65) = -1; nu(22,54) = 1;
nu(23,3) = -4; nu(23,85) = -1; nu(23,61) = 1;
nu(24,3) = -3; nu(24,54) = -1; nu(24,8) = 1;
nu(25,3) = -1; nu(25,61) = -1; nu(25,8) = 1;
nu(26,3) = -1; nu(26,86) = -1; nu(26,53) = 1;
nu(27,3) = -1; nu(27,53) = -1; nu(27,57) = 1;
nu(28,3) = -2; nu(28,57) = -1; nu(28,62) = 1;
nu(29,3) = -1; nu(29,62) = -1; nu(29,10) = 1;
nu(30,3) = -2; nu(30,116) = -1; nu(30,88) = 1;
nu(31,3) = -2; nu(31,87) = -1; nu(31,76) = 1;
nu(32,3) = -2; nu(32,76) = -1; nu(32,79) = 1;
nu(33,3) = -3; nu(33,79) = -1; nu(33,72) = 1;
nu(34,3) = -3; nu(34,72) = -1; nu(34,7) = 1;
nu(35,3) = -2; nu(35,78) = -1; nu(35,81) = 1;
nu(36,3) = -3; nu(36,81) = -1; nu(36,55) = 1;
nu(37,3) = -3; nu(37,55) = -1; nu(37,9) = 1;
nu(38,3) = -3; nu(38,84) = -1; nu(38,58) = 1;
nu(39,3) = -3; nu(39,58) = -1; nu(39,11) = 1;
nu(40,3) = -2; nu(40,60) = -1; nu(40,64) = 1;
nu(41,3) = -1; nu(41,64) = -1; nu(41,13) = 1;

% Cracking of aromatics (k(42) till k(46)
nu(42,3) = -1; nu(42,66) = -1; nu(42,4) = 1; nu(42,60) = 1; nu(42,57) = 1;
nu(43,3) = -1; nu(43,94) = -1; nu(43,69) = 1;
nu(44,3) = -1; nu(44,69) = -1; nu(44,60) = 2; nu(44,4) = 1;
nu(45,3) = -2; nu(45,83) = -1; nu(45,86) = 1; nu(45,4) = 1;
nu(46,3) = -1; nu(46,116) = -1; nu(46,87) = 1;

% HYD of S-containing components (k(47) till k(77)
nu(47,3) = -2; nu(47,67) = -1; nu(47,17) = 1;
nu(48,3) = -1; nu(48,77) = -1; nu(48,26) = 1;
nu(49,3) = -3; nu(49,26) = -1; nu(49,35) = 1;
nu(50,3) = -1; nu(50,75) = -1; nu(50,24) = 1;
nu(51,3) = -3; nu(51,99) = -1; nu(51,23) = 1;
nu(52,3) = -3; nu(52,23) = -1; nu(52,31) = 1;
nu(53,3) = -2; nu(53,109) = -1; nu(53,97) = 1;
nu(54,3) = -3; nu(54,97) = -1; nu(54,21) = 1;
nu(55,3) = -3; nu(55,21) = -1; nu(55,29) = 1;
nu(56,3) = -2; nu(56,101) = -1; nu(56,106) = 1;
```

```
nu(57,3) = -2; nu(57,106) = -1; nu(57,95) = 1;
nu(58,3) = -3; nu(58,106) = -1; nu(58,32) = 1;
nu(59,3) = -3; nu(59,95) = -1; nu(59,19) = 1;
nu(60,3) = -2; nu(60,32) = -1; nu(60,19) = 1;
nu(61,3) = -3; nu(61,19) = -1; nu(61,28) = 1;
nu(62,3) = -1; nu(62,121) = -1; nu(62,18) = 1;
nu(63,3) = -3; nu(63,18) = -1; nu(63,27) = 1;
nu(64,3) = -3; nu(64,27) = -1; nu(64,36) = 1;
nu(65,3) = -2; nu(65,111) = -1; nu(65,118) = 1;
nu(66,3) = -1; nu(66,118) = -1; nu(66,37) = 1;
nu(67,3) = -3; nu(67,37) = -1; nu(67,25) = 1;
nu(68,3) = -3; nu(68,25) = -1; nu(68,33) = 1;
nu(69,3) = -2; nu(69,102) = -1; nu(69,108) = 1;
nu(70,3) = -2; nu(70,108) = -1; nu(70,115) = 1;
nu(71,3) = -1; nu(71,108) = -1; nu(71,112) = 1;
nu(72,3) = -1; nu(72,115) = -1; nu(72,34) = 1;
nu(73,3) = -2; nu(73,112) = -1; nu(73,34) = 1;
nu(74,3) = -3; nu(74,112) = -1; nu(74,38) = 1;
nu(75,3) = -3; nu(75,34) = -1; nu(75,22) = 1;
nu(76,3) = -2; nu(76,38) = -1; nu(76,22) = 1;
nu(77,3) = -3; nu(77,22) = -1; nu(77,30) = 1;

% HYD of N-containing components (k(78) till k(84)
nu(78,3) = -2; nu(78,127) = -1; nu(78,129) = 1;
nu(79,3) = -2; nu(79,132) = -1; nu(79,126) = 1;
nu(80,3) = -2; nu(80,126) = -1; nu(80,128) = 1;
nu(81,3) = -2; nu(81,50) = -1; nu(81,52) = 1;
nu(82,3) = -2; nu(82,52) = -1; nu(82,41) = 1;
nu(83,3) = -2; nu(83,43) = -1; nu(83,48) = 1;
nu(84,3) = -2; nu(84,39) = -1; nu(84,44) = 1;

% Cracking part two (k(85) till (k(94)
nu(85,3) = -1; nu(85,87) = -1; nu(85,86) = 2;
nu(86,3) = -2; nu(86,107) = -1; nu(86,86) = 1; nu(86,92) = 1;
nu(87,3) = -1; nu(87,7) = -1; nu(87,10) = 2;
nu(88,3) = -1; nu(88,9) = -1; nu(88,10) = 1; nu(88,13) = 1;
nu(89,3) = -1; nu(89,11) = -1; nu(89,13) = 2;
nu(90,3) = -1; nu(90,78) = -1; nu(90,86) = 1; nu(90,60) = 1;
nu(91,3) = -1; nu(91,84) = -1; nu(91,60) = 2;
nu(92,3) = -2; nu(92,51) = -1; nu(92,4) = 1; nu(92,46) = 1; nu(92,60) = 1;
nu(93,3) = -2; nu(93,47) = -1; nu(93,14) = 1;
nu(94,3) = -2; nu(94,68) = -1; nu(94,14) = 1;

% HDS and HDN reactions (k(95) and k(117)
nu(95,3) = -2; nu(95,17) = -1; nu(95,4) = 1; nu(95,1) = 1;
nu(96,3) = -3; nu(96,35) = -1; nu(96,10) = 1; nu(96,4) = 1; nu(96,1) = 1;
nu(97,3) = -3; nu(97,24) = -1; nu(97,57) = 1; nu(97,4) = 1; nu(97,1) = 1;
nu(98,3) = -3; nu(98,31) = -1; nu(98,13) = 3; nu(98,1) = 1;
nu(99,3) = -3; nu(99,29) = -1; nu(99,13) = 1; nu(99,10) = 1; nu(99,1) = 1;
nu(100,3) = -3; nu(100,28) = -1; nu(100,10) = 2; nu(100,1) = 1;
nu(101,3) = -5; nu(101,36) = -1; nu(101,13) = 2; nu(101,4) = 2; nu(101,1) =
2;
nu(102,3) = -5; nu(102,33) = -1; nu(102,10) = 1; nu(102,13) = 1; nu(102,4)
= 1; nu(102,1) = 2;
nu(103,3) = -5; nu(103,30) = -1; nu(103,10) = 2; nu(103,4) = 1; nu(103,1) =
2;
nu(104,3) = -2; nu(104,123) = -1; nu(104,116) = 1; nu(104,1) = 1;
nu(105,3) = -2; nu(105,20) = -1; nu(105,4) = 2; nu(105,1) = 1;
nu(106,3) = -1; nu(106,40) = -1; nu(106,14) = 1; nu(106,2) = 1;
nu(107,3) = -4; nu(107,49) = -1; nu(107,4) = 1; nu(107,2) = 1;
nu(108,3) = -2; nu(108,130) = -1; nu(108,84) = 1; nu(108,2) = 1;
```

```
nu(109,3) = -4; nu(109,125) = -1; nu(109,60) = 1; nu(109,4) = 1; nu(109,2)
= 1;
nu(110,3) = -2; nu(110,129) = -1; nu(110,81) = 1; nu(110,2) = 1;
nu(111,3) = -2; nu(111,128) = -1; nu(111,79) = 1; nu(111,2) = 1;
nu(112,3) = -4; nu(112,131) = -1; nu(112,4) = 1; nu(112,54) = 1; nu(112,2)
= 1;
nu(113,3) = -4; nu(113,124) = -1; nu(113,4) = 1; nu(113,57) = 1; nu(113,2)
= 1;
nu(114,3) = -2; nu(114,41) = -1; nu(114,14) = 1; nu(114,4) = 1; nu(114,2) =
1;
nu(115,3) = -4; nu(115,46) = -1; nu(115,12) = 1; nu(115,2) = 1;
nu(116,3) = -5; nu(116,44) = -1; nu(116,14) = 1; nu(116,2) = 1;
nu(117,3) = -6; nu(117,51) = -1; nu(117,60) = 1; nu(117,4) = 1; nu(117,2) =
1;

% Crack reactions S-containing components (special cases K(118) till
% k(129)
nu(118,3) = -8; nu(118,93) = -1; nu(118,79) = 1; nu(118,1) = 2;
nu(119,3) = -8; nu(119,96) = -1; nu(119,81) = 1; nu(119,1) = 2;
nu(120,3) = -8; nu(120,98) = -1; nu(120,84) = 1; nu(120,1) = 2;

% Special crack and isomerization reactions k(121) till k(138)
nu(121,14) = -1; nu(121,15) = 1;
nu(122,15) = -1; nu(122,16) = 1;
nu(123,3) = -5; nu(123,6) = -1; nu(123,14) = 2; nu(123,4) = 1;
nu(124,3) = -6; nu(124,7) = -1; nu(124,14) = 1; nu(124,4) = 1;
nu(125,3) = -4; nu(125,8) = -1; nu(125,14) = 1; nu(125,4) = 1;
nu(126,3) = -5; nu(126,9) = -1; nu(126,14) = 1; nu(126,4) = 1;
nu(127,3) = -3; nu(127,10) = -1; nu(127,14) = 1; nu(127,4) = 1;
nu(128,3) = -3; nu(128,11) = -1; nu(128,14) = 1; nu(128,4) = 2;

nu(129,3) = -8; nu(129,41) = -1; nu(129,14) = 1;
nu(130,3) = -2; nu(130,90) = -1; nu(130,92) = 1; nu(130,4) = 1;
nu(131,3) = -13; nu(131,45) = -1; nu(131,60) = 1; nu(131,14) = 1;
nu(132,3) = -2; nu(132,48) = -1; nu(132,50) = 1; nu(132,4) = 1;
nu(133,3) = -4; nu(133,74) = -1; nu(133,54) = 1; nu(133,4) = 1; nu(133,1)=
1;
nu(134,3) = -1; nu(134,76) = -1; nu(134,57) = 1; nu(134,86) = 1;
nu(135,3) = -2; nu(135,113) = -1; nu(135,92) = 1; nu(135,1) = 1;
nu(136,3) = -4; nu(136,119) = -1; nu(136,104) = 1; nu(136,4) = 1;
nu(137,3) = -4; nu(137,104) = -1; nu(137,113) = 1; nu(137,4) = 1;
nu(138,3) = -2; nu(138,88) = -1; nu(138,86) = 1; nu(138,57) = 1;

% Create a sparse stoichiometric matrix:
nu = sparse(nu);
```

- Run_RX2_RX3.m:

```
% The file run_RX2_RX3.m should be run to calculate the molar flow profile
% in reactor RX2 and RX3. It loads import.mat andd uses RX2fun_tot.m
% RX3fun.m. These file use dfdV_all.m and stoich.m and reac.m will be used
% by dfdV_all.m.

clear all
format compact
format short e

global z rho phi_m_in phi_m_end K Mwt wt_per_in wt_per_end phi_end
h2_quench n
```

```
load import.mat

h2_in = 7.85e3;

% wt_per_in is loaded

% Mass flows leaving the reactor
% H2S, NH3, H2, light gas
m1 = 1;
mass_H2S0 = RX2(m1,2)*Mwt(1,1);
mass_NH30 = RX2(m1,3)*Mwt(2,1);
mass_H20 = RX2(m1,4)*Mwt(3,1);
mass_lg0 = RX2(m1,5)*Mwt(4,1);

mass_gas_in = [mass_H2S0;mass_NH30;mass_H20;mass_lg0];

% k is loaded
param(1:n) = k(1:n);

% The molar flows at the inlet of the reactor RX2
phi0 = ([mass_gas_in;phi_m_in/100*wt_per_in]./Mwt);

[RX2,m1,m2] = RX2fun_tot(phi0,param);

% The molar flows at the inlet of the reactor RX3
phi0 = RX2(m1,2:m2);

% Because of the semi countercurrent mode of operation H2S, NH3 and light
% gas are not present. Fresh H2 is added, 5.6 [ton/h]
phi0(1,1:4) = [0;0;h2_in/0.002;0]'; % [mol/h], 5.6 [ton/h] H2

[RX3,m3,m4] = RX3fun(phi0,param);

mass_H2S = RX3(m3,2)*Mwt(1,1);
mass_NH3 = RX3(m3,3)*Mwt(2,1);
mass_H2 = RX3(m3,4)*Mwt(3,1);
mass_lg = RX3(m3,5)*Mwt(4,1);

error          =          [(mass_H2S-mass_H2S0)/mass_H2S;(mass_NH3-
mass_NH30)/mass_NH3;(mass_H2-mass_H20)/mass_H2;(mass_lg-mass_lg0)/mass_lg];

mass_H2S0 = mass_H2S;
mass_NH30 = mass_NH3;
mass_H20 = mass_H2;
mass_lg0 = mass_lg;

while error(1,1) > 1e-6 || error(2,1) > 1e-6 || error(3,1) > 1e-6 ||
error(4,1) > 1e-6
    % Change the mass flows of H2S, NH3, H2 and light gas
    mass_gas_in = [mass_H2S0;mass_NH30;mass_H20;mass_lg0];
    % The molar flows at the inlet of the reactor RX2
    phi0 = [mass_gas_in;phi_m_in/100*wt_per_in]./Mwt;

    [RX2,m1,m2] = RX2fun_tot(phi0,param);

    % The molar flows at the inlet of the reactor RX3
    phi0 = RX2(m1,2:m2)';
    %Fresh H2 is added, 5.6 [ton/h]
```

```
    phi0(1:4,1) = [0;0;h2_in/0.002;0]; % [mol/h]

    [RX3,m3,m4] = RX3fun(phi0,param);

    for i = 1:m3
        S_factor = Mwt(5:m4-1,1).*Scontent;
        S_mass = RX3(i,6:m4)*S_factor;
        HC_mass = RX3(i,6:m4)*Mwt(5:m4-1,1);
        if S_mass/HC_mass <= 2.25e-4
            mass_H2S = RX3(m3,2)*Mwt(1,1);
            mass_NH3 = RX3(m3,3)*Mwt(2,1);
            mass_H2 = RX3(m3,4)*Mwt(3,1);
            mass_lg = RX3(m3,5)*Mwt(4,1);

            error = [(mass_H2S-mass_H2S0)/mass_H2S;(mass_NH3-
mass_NH30)/mass_NH3;(mass_H2-mass_H20)/mass_H2;(mass_lg-mass_lg0)/mass_lg];

            mass_H2S0 = mass_H2S;
            mass_NH30 = mass_NH3;
            mass_H20 = mass_H2;
            mass_lg0 = mass_lg;

            row = i;
            break
        elseif (i == m3) && (S_mass/HC_mass > 2.25e-4)
            disp('Catalyst bed volume is too small')
            disp('At the end of the catalyst bed with a volume of:')
            disp(RX3(m3,1)
            disp('the total massstream of sulphur is:')
            disp(S_mass)
            disp('That is in ppm wt S;')
            disp(S_mass/HC_mass)
            return
        end
    end
end

% Saving the results in a txt file
file = fopen('results2.txt', 'w');
for i = 1:m1
    fprintf(file, '%15.7f\n', RX2(i,:);
end
fclose(file);
file = fopen('results3.txt', 'w');
for i = 1:m3
    fprintf(file, '%15.7f\n', RX3(i,:);
end
fclose(file);

% Volume of RX2:
V_RX2 = RX2(m1,1);

% Volume of RX3 needed for 225 ppm S
V_RX3 = RX3(row,1);

% Sulphur content after RX2:
S_factor_RX2 = Mwt(5:(m2-1),1).*Scontent;
S_mass_RX2 = RX2(m1,6:m2)*S_factor_RX2;
S_wt_per_RX2 = S_mass_RX2*100/(RX2(m1,6:m2)*Mwt(5:m2-1,1);
```

```
% Sulphur content after RX3:
S_factor = Mwt(5:(m4-1),1).*Scontent;
S_mass = RX3(row,6:m4)*S_factor;
S_wt_per = S_mass*100/(RX3(row,6:m4)*Mwt(5:m4-1,1);

% Nitrogen content after RX2:
N_factor_RX2 = Mwt(5:(m2-1),1).*Ncontent;
N_mass_RX2 = RX2(m1,6:m2)*N_factor_RX2;
N_wt_per_RX2 = N_mass_RX2*100/(RX2(m1,6:m2)*Mwt(5:m2-1,1);

% Nitrogen content after RX3:
N_factor = Mwt(5:(m4-1),1).*Ncontent;
N_mass = RX3(row,6:m4)*N_factor;
N_wt_per = N_mass*100/(RX3(row,6:m4)*Mwt(5:m4-1,1);

% H2 RX2 out:
h2_rec = RX2(m1,4)*Mwt(3,1);

% Display the results on screen:
disp('The volumes of RX2 and RX3 in m^3 catalyst bed are:')
disp(V_RX2)
disp(V_RX3)

disp('The sulphur contents after RX2 and RX3 in wt% are:')
disp(S_wt_per_RX2)
disp(S_wt_per)

disp('The nitrogen contents after RX2 and RX3 in wt% are:')
disp(N_wt_per_RX2)
disp(N_wt_per)

disp('The hydrogen entering RX3 is:')
disp(h2_in)

disp('The hydrogen leaving RX2 is:')
disp(h2_rec)

disp('The hydrogen quench of RX2 and RX3 in total is:')
if V_RX3 < 16
    disp(h2_quench*4*Mwt(3,1)
    quench = 0;
elseif V_RX3 >= 16 && V_RX3 < 64
    disp(h2_quench*4*Mwt(3,1)+1.25e3)
    quench = 1.25e3;
elseif V_RX3 >= 64 && V_RX3 < 128
    disp(h2_quench*4*Mwt(3,1)+2.25e3)
    quench = 2.25e3;
elseif V_RX3 >= 128
    disp(h2_quench*4*Mwt(3,1)+3e3)
    quench = 3e3;
end

% H2 consumption
H2_cons = h2_in + quench + 4*h2_quench*Mwt(3,1) - RX2(m1,4)*Mwt(3,1);

disp('The hydrogen consumption of RX2 and RX3 in total is:')
disp(H2_cons)
```

```
% Produce figure of H2 profile
figure(1)
subplot(2,1,1), plot(RX2(:,1),RX2(:,4))
title('Molar flow profile in RX2')
xlabel('Volume of catalyst bed /[m^3]')
ylabel('Molar flows of H2 /[mol/h]')

subplot(2,1,2), plot(RX3(1:row,1),RX3(1:row,4)
xlabel('Volume of catalyst bed /[m^3]')
ylabel('Molar flows of H2 /[mol/h]')

% Save results in a workspace
savefile = 'results.mat';
save(savefile, '-mat');
```

- RX2fun_tot.m:

```
function [RX2,m1,m2] = RX2fun_tot(phi0,param)

global  z  rho  phi_m_in  phi_m_end  K  Mwt  wt_per_in  wt_per_end  phi_end
h2_quench n

% Options for the integration
options = odeset('AbsTol', 1e-6, 'RelTol', 1e-4);

% Boundary conditions and domain
V0 = 0;                  % [m^3] initial volume
V1 = 12.5;               % [m^3] volume of first catalyst bed
V2 = 12.5 + 32;          % [m^3] volume of second catalyst bed
V3 = 12.5 + 2 * 32;      % [m^3] volume of third catalyst bed
Vf = 12.5 + 3 * 32;      % [m^3] volume of fourth catalyst bed

% First integration
Vspan = [V0 V1];         % integration domain
phi0(3,1) = phi0(3,1) + h2_quench;
[V,phi] = ode113('dfdV_all', Vspan, phi0, options, param);
bed1 = [V,phi];

% Second integration
Vspan = [V1 V2];         % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench;
phi0 = phi(length(V),:);
[V,phi] = ode113('dfdV_all', Vspan, phi0, options, param);
bed2 = [V,phi];

% Third integration
Vspan = [V2 V3];         % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench;
phi0 = phi(length(V),:);
[V,phi] = ode113('dfdV_all', Vspan, phi0, options, param);
bed3 = [V,phi];

% Fourth integration
Vspan = [V3 Vf];         % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench;
phi0 = phi(length(V),:);
[V,phi] = ode113('dfdV_all', Vspan, phi0, options, param);
bed4 = [V,phi];

% Save results in one matrix
```

```
RX2 = [bed1;bed2;bed3;bed4];

% Size of the matrix
[m1,m2] = size(RX2);
```

- RX3fun.m:

```
function [RX3,m3,m4] = RX3fun(phi0,param)

global  z  rho  phi_m_in  phi_m_end  K  Mwt  wt_per_in  wt_per_end  phi_end
h2_quench n

% Options for the integration
options = odeset('AbsTol', 1e-5, 'RelTol', 1e-5);

h2_quench2 = 1250/0.002;         % [mol/h], total quench is about 3 [ton/h]
h2_quench3 = 1000/0.002;
h2_quench4 = 750/0.002;

% The reactor volume
V0 = 0;
V1 = 16;
V2 = 64;
V3 = 128;
V4 = 192;

% First integration
Vspan = [V0 V1];         % integration domain
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);
bed1 = [V,phi];

% Second integration
Vspan = [V1 V2];         % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench2;
phi0 = phi(length(V),:);
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);
bed2 = [V,phi];

% Third integration
Vspan = [V2 V3];         % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench3;
phi0 = phi(length(V),:);
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);
bed3 = [V,phi];

% Fourth integration
Vspan = [V3 V4];         % integration domain
phi(length(V),3) = phi(length(V),3) + h2_quench4;
phi0 = phi(length(V),:);
[V,phi] = ode45('dfdV_all', Vspan, phi0, options, param);
bed4 = [V,phi];

% Save results in one matrix
RX3 = [bed1;bed2;bed3;bed4];

% Size of the matrix
[m3,m4] = size(RX3);
```

15.7.6 Results for kinetic parameters in Matlab®

Table 15.20 Kinetic parameters and mass flows leaving (R02) and (R03)

		R02	R03
k	Component ID	[ton/h]	[ton/h]
2.00E-01	H2S	7.71E+00	1.23E+00
7.30E-02	NH3	8.01E-01	1.88E-01
7.30E-02	H2	4.32E+00	5.60E+00
5.00E-02	light gas	1.94E+01	7.85E+00
5.00E-02	2f1	5.42E+00	9.04E+00
3.50E-01	3f1	2.53E+00	1.10E+00
3.50E-01	3f2	1.17E-02	2.19E-08
2.18E-01	4f1	4.23E+00	3.69E-01
5.50E-02	4f2	3.48E+00	7.56E+00
1.55E-01	5f1	7.35E+00	6.62E-01
2.40E-01	5f2	1.22E+00	2.00E+00
1.18E-01	6f1	2.34E+00	2.41E+00
5.00E-02	6f2	2.06E+01	2.57E+01
5.00E-02	7f1	1.24E+01	3.44E+00
4.75E-01	7f2	1.13E+01	3.02E+01
8.10E-02	7f3	2.41E+00	2.14E+01
7.70E-02	1g1	1.59E-02	2.03E-09
7.80E-02	1g2	1.69E-02	1.22E-03
2.70E-01	1g3	1.69E-02	3.66E-05
2.70E-01	2g1	2.20E-02	5.04E-07
9.00E-03	2g2	2.27E-02	1.88E-04
8.00E-01	2g3	2.28E-02	6.02E-05
9.00E-03	3g1	1.64E-02	3.16E-08
3.95E-01	3g2	1.72E-02	1.49E-03
8.60E-02	3g3	1.69E-02	1.35E-04
7.40E-02	4g1	1.66E-02	4.37E-06
9.10E-02	4g2	1.69E-02	1.22E-03
1.08E-01	4g3	1.69E-02	3.66E-05
3.04E+00	5g1	1.77E-02	1.47E-04
2.05E-01	5g2	1.78E-02	4.71E-05
1.20E-03	6g1	1.24E-02	2.39E-08
4.15E-02	6g2	1.28E-02	2.78E-05
5.00E-02	6g3	1.26E-02	1.01E-04
0	6g4	1.28E-02	3.35E-05
2.70E-01	7g1	1.12E-02	2.95E-06
1.70E-01	7g2	1.13E-02	8.20E-04
3.10E-01	7g3	1.13E-02	9.09E-05
3.10E-02	7g4	1.15E-02	3.05E-05
1.00E-02	1i1	6.21E-02	1.02E-04
2.20E-01	1i2	6.21E-02	1.02E-04
3.80E+00	2i1	9.88E-02	2.62E-04
4.34E-01	2i2	1.36E-10	1.36E-10
2.30E-01	2i3	9.77E-02	2.54E-04
4.75E-01	3i1	7.63E-02	1.30E-04
1.00E-02	3i2	7.76E-02	2.02E-04
2.05E-01	4i1	5.07E-02	1.23E-04
5.20E-01	4i2	5.09E-02	1.85E-04
2.70E-01	4i3	5.01E-02	1.31E-04
5.10E+00	5i1	4.56E-02	7.97E-05
8.00E-02	5i2	4.56E-02	1.19E-04
4.31E-01	6i1	1.23E-01	2.75E-04
4.95E+00	7i1	1.36E-01	3.58E-04
1.57E-01	1a1	1.21E+00	4.42E-01
2.80E+00	1a2	1.15E+00	6.89E-02
3.00E+00	1a3	1.21E+00	3.21E-02
2.01E-01	1a4	1.20E+00	5.10E-01
2.04E-01	2a1	3.65E+00	7.96E-01
2.04E-01	2a2	2.49E+00	2.73E+00
7.20E-01	2a3	3.65E+00	9.91E-01
4.51E+00	3a1	3.00E+00	7.36E-03
8.27E+00	3a2	2.04E+00	3.32E-01
8.60E-02	4a1	1.35E-01	2.96E-02
2.53E+00	4a2	1.28E-01	2.53E-03
2.68E+00	5a1	1.91E-01	4.72E-04
1.57E-01	5a2	1.89E-01	1.10E-02
5.95E-01	5a3	1.83E-01	3.22E-07
7.56E+00	6a1	1.15E-01	1.47E-08
5.36E+00	6a2	2.41E-01	7.59E-07
2.01E-01	6a3	2.40E-01	8.92E-05
2.06E-01	6a4	2.43E-01	4.95E-02
2.06E-01	7a1	9.61E-01	4.70E-02
3.19E-01	7a2	5.95E-01	2.23E+00
1.54E-01	7a3	6.02E-01	1.06E+00
1.54E-01	1b1	9.47E-03	5.53E-11
1.47E+01	2b1	4.57E-01	3.97E-02
5.76E+00	2b2	4.52E-01	4.93E-02
1.15E+01	3b1	2.93E-01	7.71E-05
2.10E-01	3b2	2.93E-01	7.68E-05
2.05E-01	4b1	1.38E+00	5.67E-01
4.10E-01	4b2	9.61E-01	4.01E-01
6.83E-01	5b1	2.01E+00	2.82E-02
4.28E-01	5b2	5.73E-01	9.98E-02

k	Component ID	R02 [ton/h]	R03 [ton/h]
1.95E-01	6b1	3.17E-01	2.34E-01
2.10E-01	6b2	1.51E+00	6.67E-01
1.20E-03	6b3	1.54E+00	1.68E+00
2.01E-01	7b1	8.12E-01	3.14E-01
4.32E-01	7b2	8.18E-01	1.01E+00
1.00E-03	1c1	8.88E-01	1.09E-01
1.50E-03	2c1	1.30E+00	1.08E-01
1.00E-04	3c1	8.48E-01	1.87E-01
1.00E-04	3c2	8.32E-01	1.92E-02
1.00E-01	4c1	4.40E-01	2.95E-02
1.84E-01	4c2	4.42E-01	1.64E-02
4.15E-01	5c1	1.05E-01	9.38E-05
4.46E+00	5c2	1.06E-01	2.29E-04
8.16E+00	5c3	1.05E-01	9.38E-05
2.23E+00	6c1	2.25E-02	1.87E-04
7.20E+00	6c2	2.13E-02	2.59E-10
4.10E+00	7c1	1.66E-01	3.21E-07
8.65E+00	1d1	2.72E-01	6.06E-04
4.17E+00	1d2	2.70E-01	5.84E-04
7.47E+00	1d3	2.70E-01	5.84E-04
1.51E+01	2d1	4.71E-01	4.36E-02
8.60E-02	2d2	4.76E-01	4.85E-03
3.50E-01	2d3	4.75E-01	4.52E-02
2.10E-01	3d1	2.65E-01	5.75E-04
2.08E-01	3d2	2.62E-01	5.67E-04
2.17E-01	3d3	2.61E-01	5.63E-04
2.20E-01	4d1	3.73E-01	3.09E-03
7.40E-01	4d2	1.13E+00	1.13E+00
9.50E-01	4d3	3.73E-01	3.09E-03
2.05E-01	4d4	3.72E-01	9.82E-04
2.15E-01	5d1	3.79E-01	4.75E-03
3.88E-01	5d2	3.75E-01	3.30E-03
3.05E-01	5d3	3.78E-01	9.89E-04
3.80E-01	6d1	1.40E-01	8.16E-03
1.00E-01	6d2	6.90E-01	6.90E-01
1.08E-01	6d3	1.40E-01	1.12E-03
2.30E-01	6d4	1.42E-01	1.47E-04
5.97E-01	7d1	8.70E-01	8.70E-01
4.25E+05	7d2	4.75E-01	3.44E-02
7.25E+04	7d3	4.73E-01	5.96E-03
1.08E-01	7d4	4.75E-01	3.44E-02
0	1e1	3.30E-02	4.65E-05

k	Component ID	R02 [ton/h]	R03 [ton/h]
2.05E-01	2e1	1.11E-01	1.35E-04
0	2e2	1.11E-01	2.06E-04
2.02E-01	3e1	4.16E-01	6.83E-04
0	4e1	6.29E-02	1.15E-04
4.05E-01	5e1	1.67E-01	2.76E-04
7.70E-02	6e1	1.89E-01	2.51E-04
1.95E-01	7e1	1.06E-01	2.03E-04
5.80E-01	7e2	1.06E-01	2.03E-04
6.21E-01	Total	1.58E+02	1.37E+02
4.15E-02	Component ID based on the provided		
3.00E-01	component distribution:		
2.25E-01	first number is column number		
1.70E-01	letter gives the row		
8.90E-02	second number gives component		