Final report

CPD NR 3294
Conceptual Process Design

Process Systems Engineering
DelftChemTech - Faculty of Applied Sciences
Delft University of Technology

Subject

Design of a plant producing 500,000 tonnes/annum synthetic oil products from natural gas, using Fischer-Tropsch technology

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Summary

In this report the conceptual design of a Fischer-Tropsch plant that produces 500,000 tonne/year of synthetic fuels from natural gas is presented. A team of 3 students has carried out the conceptual process design. The design work is carried out in the framework of the course Conceptual Process Design (CPD, st4931). The assignment is to design a plant producing 500,000 tonnes/annum synthetic oil products (naphtha, kerosene and diesel) from natural gas, using Fischer-Tropsch technology. The main products must be diesel and kerosene.

The design is intended as a comparison to an alternative design made in the past. Therefore, price levels related to before 1999 should be used. In addition only literature information regarding conversion technologies from 1998 and before should be used. Any information regarding technical developments after 1998 should be discarded. This will allow a fair comparison between the present design and the alternative design. The comparison between the two processes is not included in this report.

The general design method that is used is the Delft Design Matrix (DDM) [Grievink, 2001]. The DDM is a design method that gives guidance to the design teams throughout the whole design process. The DDM is divided into 8 different design spaces that on its turn consist of 7 generic cycles (scope of design, knowledge of objects, synthesis, analysis, evaluation, report and finally go or no-go). The separation of the design process in these subspaces gives more room for implementing creativity and induces a more efficient approach. Other design tools that are used are PIQUAR, planning tools and creativity tools. The creativity tools that were used most effectively were brainstorming, TRIZ (avoiding compromises), visualization, good working atmosphere and using different ‘hats’ to judge alternatives.

The economic viability of the FT process depends on the availability of feedstock (coal or natural gas) and on the price of petroleum. High petroleum prices are favorable for the competitiveness of the FT process. In 1994, the production of synfuels, even at low natural gas prices was not considered viable by Rostrup-Nielsen at crude oil prices below US$ 30 per barrel. In the future, when petroleum sources will become more and more scarce, FT will be an option for the production of fuels and chemical feedstock for the petrochemical industry. The economic sensitivity analysis of our process showed that the prices of the products have to increase with approximately 60% or the feedstock prices of the natural gas have to decrease with approximately 50%, to reach break even. Nowadays, the production of high-value chemicals, together with transportation fuels, can make a FT plant economically viable. The general demand for low sulfur and nitrogen transport fuels can enhance the viability of the FT process, because

the produced hydrocarbons do not contain sulfur or nitrogen. Moreover the linear hydrocarbons that are produced make an excellent diesel fuel (high cetane number). The economic lifetime of the plant is determined to be 15 years and the plant is on-stream for 8000 hours/year.

The basis of the design consists of a synthesis gas production section, a Fischer-Tropsch reaction section and a product workup section. The synthesis gas from natural gas is produced with an autothermal reactor. For the Fischer-Tropsch reaction a slurry reactor is used. The product workup sections consist of a hydrocracker that cracks the heavy hydrocarbons to lighter hydrocarbons (diesel and kerosene) and an isomerization reactor that isomerizes the linear alkanes to lower the cloud and pour point of the diesel as well as the freeze point of kerosene. Two membranes, a number of gas/liquid separators and three distillation columns carry out the separations.

The most important solutions for key design problems are:

- Autothermal reforming technology is used to produce synthesis gas.
- A slurry reactor with a cobalt catalyst is used to produce hydrocarbons from synthesis gas.
- Product isomerization of kerosene and diesel is accomplished in an isomerization reactor.
- Hydrocracking the Fischer-Tropsch wax in a trickle flow hydrocracker increases middle distillate yields.
- Recycling of carbon dioxide and synthesis gas is combined. The separation is carried out by the distillation columns that also separate the final products.
- The hydrocarbons that are in the desired product range are prevented from entering the hydrocracker.
- The H_2/CO ratio of the syngas is controlled with the CO_2 recycle.

The overall heat and mass balance is shown in the table below.

Table 1: Overall heat and mass balance

	Mass in [kt/a]	**Mass out [kt/a]**
Natural gas	787.0	
Oxygen in ATR	926.2	
Oxygen in burner	296.2	
Water/steam	23.2	985.0
CO_2		536.0
Naphtha		117.8
Kerosene		187.3
Diesel		196.0
Wax		1.8
H_2 purge		1.5

N_2 out		7.1
Total	2032.6	2032.5
	Enthalpy in [MW]	**Enthalpy out [MW]**
	-549	-2520

The total yield of the FT reactor is 92%. From Table 1 is clear that large amounts of heat are generated. It is estimated that the amount of steam could be an extra income, which is comparable to the income from diesel or kerosene. This is one of the main advantages of the process; the production of synthetic oils can be combined with the production of power.

The heat integration is carried out only for the large streams in the process. The ATR effluent stream is used to heat most of the cold streams (89% of the heat streams that are taken into account is supplied by the ATR reactor effluent). The consequence of this design decision is that for start-up an additional heat source is necessary. The equipment design for the process is carried out to a minor degree of detail due to time constraint and the large amounts of units. The Fischer-Tropsch reactor is modeled in detail, but for the ATR, hydrocracker, isomerization reactor and distillation columns only the most important features are determined.

The DOW fire and explosion index is used to identify the main fire and explosion risks in the process. The ATR turned out to be the most dangerous unit in the process with an index of approximately 150, which corresponds to a heavy degree of harm. Furthermore a HAZOP study is carried out at the end of the design process. Possible weak points of the control schemes are identified in order to improve the safety of the process. A crucial scheme concerns the cooling system of the FT reactor.

At the end of the report some recommendations from the team are given, which could improve the design of the process. The most important recommendation is the recovery of the LPG from the recycle stream. In the present design all the LPG is burned in the ATR. This is not only very uneconomical, but also not very sustainable. The economic potential of the LPG recovery is approximately $5,600,000. Other recommendations concern the more detailed modeling of certain units in the process. This could also include the need of experiments and/or patents.

At the end of the project the team was asked to write an addendum. This addendum contains a revised summary and economic part, which are included in this report, and a fingerprint of the process that shows the main yields. This addendum is available on cd and as hard copy.

Table of contents

1 Introduction

The Conceptual Process Design is part of the 4th year's curriculum for students studying Process Technology at the DelftChemTech Department of the faculty of Applied Sciences at Delft Technical University. The assignment is to design a plant producing 500,000 tonnes/annum synthetic oil products from natural gas, using Fischer-Tropsch technology. The main products must be diesel and kerosene. Naphtha and LPG are accepted as by-products.

The Fischer Tropsch (FT) process was named after F. Fischer and H. Tropsch who invented the process in 1923. They showed that synthesis gas could be converted catalytically into a wide range of hydrocarbons and/or alcohols. A Fischer-Tropsch synthesis as a basis for diesel and kerosene is nowadays only limited to special cases. The general demand for sulphur free gasoline and the insecure oil market could shift this operating regime. It is expected that the ultimate role for Fischer-Tropsch synthesis lies in the production of transportation fuels [Xu, 1998].

The process consists basically of three sections: the synthesis gas production section, the Fischer-Tropsch synthesis sections and the product workup section. Naphtha is considered as a by-product of the process. Further treatment of naphtha by, for example, isomerization is not necessary, as it does not have to fulfill product requirements. The in- and outgoing streams of the process are shown in Figure 1.

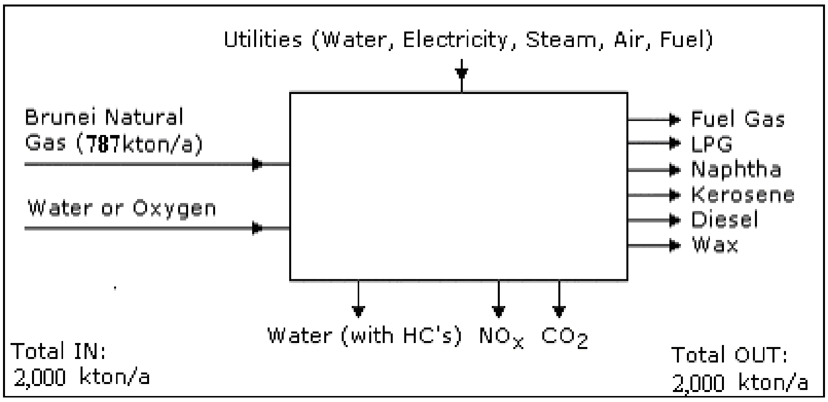

Figure 1: Input/output diagram process

Literature research was done before choosing a process or a reactor type. Based on data from literature, analysis of the technology and intuition, we have made choices for what we believe are the best options for this process. The evaluation of technologies will be treated apart for each unit. For each of them, a qualitative judgment was done in order to help us making the right decision. The most important decisions that were made for the applied technologies are:

- Autothermal reforming technology is used to produce synthesis gas.
- A slurry reactor with a cobalt catalyst is used to produce hydrocarbons from synthesis gas.
- Product isomerization of kerosene and diesel is accomplished in an isomerization reactor.
- Hydrocracking the Fischer-Tropsch wax in a trickle flow hydrocracker increases middle distillate yields.

The mentioned technologies are already applied in nowadays industry. The consequence is that much of the design data (especially equipment design) is readily available in patent literature. Some pieces of equipment for the key technologies are designed according to rough estimations by comparing the technology to an industrial comparable piece of equipment. This is the case for equipment that is based on reactions from which the team does not have detailed kinetic models (e.g. for the hydrocracker). Other pieces of equipment are designed with a model, because the reaction kinetics are known (e.g. the Fischer-Tropsch reactor). Reference is made to (patent) literature for more detailed design of equipment.

The most important solutions for key design problems are:

- Recycling of carbon dioxide and synthesis gas is combined. The separation is carried out by the distillation columns that also separate the final products.
- The cracking of hydrocarbons that are in the desired product range are prevented from entering the hydrocracker.
- The H_2/CO ratio of the syngas is controlled with the CO_2 recycle.

Sustainability has been an important issue throughout the design process. For important decisions sustainability is included as a criteria. The largest waste streams of the process consist of water and CO_2. Smaller waste streams are a wax stream and emissions of NO_X. The wastewater has to be treated by a wastewater treatment plant because of the hydrocarbons that are present in the flow. The fuels that are produced by the process are more sustainable than the present fuels, because they do not contain sulfur and nitrogen.

The design will be compared to an alternative design made in the past. Therefore, price levels related to 1999 should be used. In addition only literature information regarding conversion technologies from 1998 and before should be used. Any information regarding technical developments after 1998 should be discarded. This will allow a fair comparison between the present design and the alternative design.

Nowadays, there are not many plants based on the Fischer-Tropsch technology in operation. A summary of the plants presently using this technology to produce liquid fuel is presented in Table 2.

Table 2: Summary of plants using FT-technology to produce liquid fuels

Company	Location	Feedstock	Main products	Production (kt/a)
Sasol	South-Africa	Coal	Gasoline, Wax	4,200
Mobil*	New Zealand	Natural Gas	Gasoline	600
Mossgas	South-Africa	Natural Gas	Gasoline, Diesel	900
Shell	Malaysia	Natural Gas	Diesel, Kerosene, Wax	500

The economic viability of the FT process depends on the availability of feedstock (coal or natural gas) and on the price of petroleum. High petroleum prices are favorable for the competitiveness of the FT process. In 1994, the production of synfuels, even at low natural gas prices was not considered viable by Rostrup-Nielsen at crude oil prices below US$ 30 per barrel. In the future, when petroleum sources will become more and more scarce, FT will be an option for the production of fuels and chemical feedstock for the petrochemical industry. Nowadays, the production of high-value chemicals, together with transportation fuels, can make a FT plant economically viable.

The general design method that is used is the Delft Design Matrix (DDM) [Grievink, 2001]. The DDM is a design method that gives guidance to the design teams throughout the whole design process. The DDM is divided into 8 different design spaces that on its turn consist of 7 generic cycles (scope of design, knowledge of objects, synthesis, analysis, evaluation, report and finally go or no-go). The separation of the design process in these subspaces gives more room for implementing creativity and induces a more efficient approach.

The most important tools besides the DDM that were used during the design process were PIQUAR quality factors, an activity assistant to monitor the activities that need to be done, a time-line and AspenPlus11. The first three tools are described in chapter 2. Besides the design tools the team also applied creativity tools to enhance the creative input of each team member. In order to improve an existing design creativity is an essential tool to accomplish a good result. An innovative design is tried to accomplish by investigating various creativity methods at the start of the project. This is explained in more detail in chapter 2. The creativity and work process tools are evaluated in chapter 11.

The structure of the report is similar to the design spaces of the Delft Design Matrix, every chapters describes a design space. Each chapter has a summary, introduction, conclusion and literature references. The reports that give more information on a certain topic of the design space are placed at the end of the report as appendices. Reports that give only background information are also placed at the end of the report as appendices.

Design space 0: group formation & tools

1.1 Summary

The focus of this part of the report, Design space 0 (DS 0), is on the formation, organization and profiling of the group. We give further a short introduction to Delft design matrix (DDM) and creativity methods that can be applied to the DDM. A number of reports are created to support this document. These reports are available as appendices at the end of the report:

- Appendix 1 : Project description (R002)
- Appendix 2 : Group profile (E001)
- Appendix 3 : Advanced Activity Assistant (E004)
- Appendix 4 : Global time line (E005)
- Appendix 5 : Group rules (R001)
- Appendix 6 : PIQUAR (R010+R008)
- Appendix 7 : Creativity methods (R006)

1.2 Table of contents chapter 2

1.3 Introduction

For the CPD project we have to design a plant that produces 500,000ton/a of synthetic oil (diesel, kerosene and naphtha). As feedstock we should use natural gas and our plant is to be located in Brunei (South East Asia). The client stipulated the technology to be applied (Fischer-Tropsch synthesis technology). An overview of all the process specifications of the project can be found in the project description [R002]. The start of the design is given by a former CPD group.

If we take a look around us, we see that in almost every company, organization and even in households there is a structural approach to perform the duties. In the Conceptual process design there are also such kinds of structures to give guidance to the design teams. It is necessary to have such a structure because it improves the efficiency and enables the team to deliver qualitatively good designs. In the past, process design teams have been using different structural design methods [1].But the problem with these methods is that they are generally still focused on the existing unit operations and equipment. This causes designers to easily go over in creating flow sheets from existing process unit operations and equipment. So, These methods do not leave any opportunities for innovation, which make the methods lose their effectiveness for a really innovative design.

To improve the input of innovation in design, the 'PSE group' in Delft created the Delft Design Matrix (DDM) [2]. The DDM is a design method that gives guidance to the design teams throughout the whole design process. The DDM is divided into 8 different design spaces that on its turn consist of 7 generic cycles (scope of design, knowledge of objects, synthesis, analysis, evaluation, report and finally go or no-go). The separation of the design process in these subspaces gives more room for implementing creativity and induces a more efficient approach. For these reasons the DDM will be used in this design project.

1.4 Scope of design space 0

In this phase the designer defines the design space, which comprises:

- Type of objects:
  - Group formation and functioning

- Battery limits and interactions:
  - The system is the design team
  - The design team interacts with Mr. Swinkels who is the team's principal client and creativity coach. The team also interacts with mr. Ajah who is the team's PHD student assistant.
  - The design team also has interaction with a number of tools that are going to be used: creativity methods, planning tools (AAA and time-line), quality assessment with PIQUAR and the DDM

- Exchange streams with the environment:
  - Memos to the client and principal
  - Creativity meetings (once a week when we start with DS3)
  - Meetings with mr. Ajah about the DDM (once a week when we start with DS3)
  - Main deliverables (kick-off meeting, BOD, BOD review and final report)

- Feedback from client/principal and mr. Ajah after each DS

❑ Constraints:
- The design method (DDM)
- Dates for main deliverables
- Main contents and format of the memos and report as defined in the group rules and the CPD-manual [2]
- Requirements on the quality of the design [2]
- Evaluation tool (PIQUAR)
- PIQUAR quality factors (R008)

❑ Variables
- Time planning
- Use of creative tools
- Group rules
- Group strengths and weaknesses

❑ Recommending the use of certain technologies:
- Creativity tools by dr. Grunwald [4]
- PIQUAR for evaluation
- Advanced Activity Assistant (available on blackboard)
- Initial design from former CPD group

❑ Restrictions
- DS0 must be finished for kick-off meeting: 19-05-2003
- DS0 is created by 3 people

1.5 Knowledge of objects

In this phase the designer identifies a set of suitable objects for the synthesis phase and assesses the knowledge that is (not) available concerning these blocks. The tools that are used to manipulate the objects in the design are defined in this phase.

❑ Suitable objects for group functioning:
- Creativity methods, these are necessary because our aim is to generate an innovative design
- Time planning, because the project last 3 months timing is very important right from the start.
- Team capacity, weaknesses and strengths can be investigated by means of individual and group profiles and thereby maximizing the group capacity
- Group rules, certain guidelines are necessary in order to work efficient
- Design method and a quality control for the design method that is called the PIQUAR method.

- Knowledge available on these objects:
  - Creativity methods: each group member has read two articles about methods that could increase creativity. Each member has made a summary of the articles and wrote something about the implementation of these methods.
  - Time planning: the most important knowledge about the time planning are the dates for the main deliverables set by the principal/client (R002). Furthermore the team wants to deliver a report after each DS to the principal/client and receive some useful feedback.
  - Team capacities: If the team wants to function optimally and efficiently, a prerequisite is to have a group profile. There is no team without individuals. Because of this statement it is necessary to have a personal profile from each individual to be able to make a group profile [E001]. With the group profile the strengths and the weaknesses of the design team become known and these can be taken into account during the design.
  - Group rules: Another important aspect of group formation are the group rules [R001]. In the group rules the team defined some basic rules for routine tasks and a general standard for documentation.
  - The design method is already defined, the DDM [2]. The design method is evaluated with a document about the strengths and weaknesses of the DDM (R007). The quality factors for the PIQUAR evaluation are already defined by the principal and former CPD group (R008).

- Tools to manipulate the objects in the design:
  - Group meetings
  - Individual reports on creative methods and individual profile

1.6 Synthesis, analysis and evaluation

The result of each object is described in a number of reports:

- Creative methods (R006)
- Global time planning (E005)
- Advanced Activity Assistant (E004)
- Individual and group profiles (E001)

  We have noticed that planning is a weak point of the group. Therefore we agreed on making tight schedules. The team mainly uses two tools; the time-line and the Advanced Activity Assistant. The time-line is made to give an overview of the deliverables, their deadlines and the time spent in each design space. It serves as a tool to help the planning of the tasks. The Advanced Activity Assistant has the same purpose, but is a more detailed tool, with defined tasks, defined deadlines for each task, input and output of each task. These tools should be followed as close as possible and they should be updated regularly. The time-line is changed whenever the team concludes that the stated periods are not optimal and the advanced activity assistant is updated weekly by means of group meetings. Each member is also responsible for maintaining the tasks in the activity assistant (especially his own tasks).

- Group rules (R001)
- PIQUAR template and weighing factors (E003+R008)
- An input/output model of DS0 is given in Figure 2.

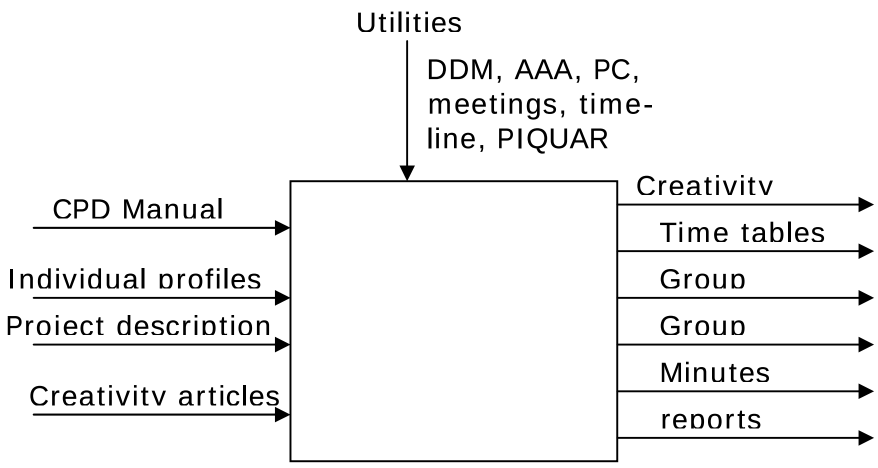

Figure 2: Blockscheme of DS 0

1.7 Conclusions

In this report the formation of our group is described. The capacity of our group is tried to increase with group rules, creativity assignments, various time planning and a group profile assessment.

1.8 Literature

1. J.M.Douglas, 1988,Conceptual Design of Chemical Processes.
2. J. Grievink et.al., 2001, A framework for conceptual design of process plants.

3. J. Grievink, C.P. Luteijn, P.L.J. Swinkels, instruction manual conceptual design, 2002, PSE-group, faculty of applied sciences, Delft university of technology.
4. D.H. Grunwald, Process conditions for using creativity in design work, 1997, faculty of chemical technology, Delft University of technology.

Design space 1: input/output structure

Summary

This report discusses the results of Design Space 1. In this level of the Delft Design Matrix (DDM, [1]) the supply chain related I/O structure is defined. The main results of this design space are discussed in this chapter. The results are further explained in reports that are included as appendices:

- Appendix 8: Feedstock, product and byproduct specifications (R101)
- Appendix 9: Dow fire & explosion indices of DS1 (R102)
- Appendix 10: Waste and byproduct specifications (R103)
- Appendix 11: Economics DS1 (R104)
- Appendix 12: European environmental legislation (R105)
- Appendix 13: Utilities and auxiliaries (R106)
- Appendix 14: Preliminary mass balances DS1 (R107).
- Appendix 15: Diesel additives (R108)
- Appendix 16: Quality of water (R109)
- Appendix 17: Pure component properties (E301)

The key-output of this design space is the I/O structure in Figure 3.

Contents chapter 3

1.9 Scope of Design space 1

In this phase the designer defines the Design Space, which comprises of a number of objects:

1. Type of objects to be considered:
    - Plant inside

- Facilities outside
- Storage

2. Boundaries of the system for the input/output structure
   - Natural environment
   - Suppliers and customers
   - Owning company
   - Local authorities
   - Personnel
   - Capital
   - Waste streams

3. Exchange streams with the environment:
   - Feed stock (Natural gas from Brunei)
   - Product (Diesel and Kerosene)
   - By-products (Naphtha and LPG)
   - Auxiliaries (steam, air) and utilities (steam, air, cooling water)
   - Emissions (CO_2, HC and NO_x)
   - Additives to increase product Quality

4. Constraints on, and targets for the structure, scale, and (physical) behavior of the system:
   - Function of the process is to be production of syntroleum products out of natural gas
   - Product specifications are given by the principal of the project
   - Is there a pattern in production or are there seasonal demands
   - Production of products using the Fischer-Tropsch process
   - If possible heavy by-products are preferred above light by-products. These heavy by-products are to be treated in a hydro cracker to produce diesel and kerosene
   - Location constraints including safety, environmental and infrastructure
   - Annual production hours
   - Only technical and economic data from before 1999 is to be used
   - Economic potential
   - Availability and education level of personnel
   - Availability of capital
   - Quality control using PIQUAR as agreed with principal

5. Identifying the variables that characterize the objects in the Design Space and their topology:
   - Stream compositions (concentration, pressure and temperature).
   - Feedstock reliability and availability.
   - Market price for products and by-products.
   - Mode of delivery for each stream.
   - Mode of operation (batch or continuous).
   - Annual production time

- Product split
- Annual production capacity

6. Identifying restrictions on the design stage itself with respect to manpower and time available:
   - DS 1 is done by a team of 3 students and is to be finished on Wednesday 21/05/2003
   - DS 1 is part of the Basis of Design report, that is to be submitted on Wednesday 02/06/2003

1.10 Knowledge of objects

1. Identifying suitable objects:

   The object of this Design Space, the supply chain input and output related structure, is very much restricted. The input and output for the total process are a restriction of this project. The synthesis for this Design Space shall be very limited. The feedstock and its mode of delivery, the process to be used and the output streams are already defined. The only variables to be specified are the mode of operation and the annual production time.

2. Knowledge that is available and knowledge that is not available on these objects:
   - The feed stream is completely defined by the principal and its properties are listed in R101. The mode of delivery shall be through pipeline. The feedstock is natural gas from Brunei.
   - The mode of operation for this process should be defined (R101).
   - A safety analysis should be carried out (R102).
   - The waste and byproduct streams should be investigated (R103).
   - The market price for products and by-products should be investigated (R104).
   - The EU (Dutch) emission rules are to be used. As a corporate policy, safety regulations from Europe (The Netherlands) are used. These rules are to be defined and future developments are to be examined (R105 and R109).
   - The utilities and auxiliaries are defined (R106).
   - A preliminary mass balance is set up (R107).
   - Pure component properties (E301).
   - The possible use of fuel additives is investigated (R108)

3. Tools:

   Synthesis, analysis and evaluation:
   - Not many variables need to be manipulated, so there are no tools needed for synthesis.
   - To analyze the Design Space a number of tools will be used.

- The Dow fire and explosion index shall be used to analyze the risk of this process.
- The PIQUAR tool will be used to keep an eye on the quality of the design.
- An economic evaluation will be made of the process for this Design Space.

1.11 Synthesis, Analysis and Evaluation

The synthesis for this Design Space is limited, because of the large amount of constraints on the process. The feedstock and product specifications are set and listed in R101. The input output structure of the plant concluded from reports R101 to R108 is schematically shown in Figure 3.

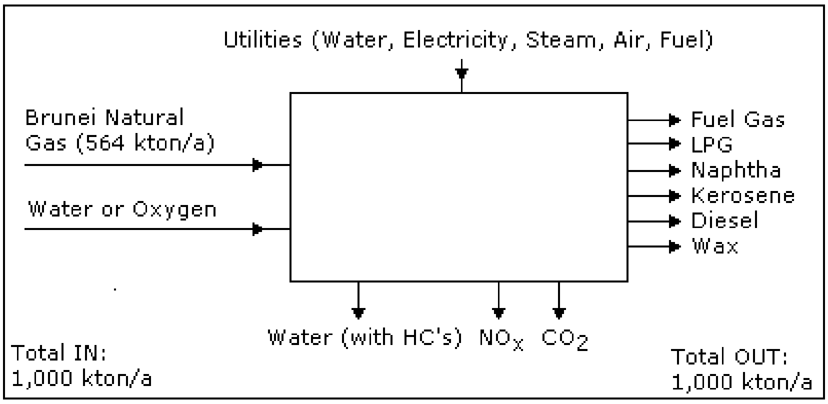

Figure 3: Input/output structure for Design Space 1

For each stream a report was written. Furthermore the legislation for emissions was examined. For the analysis of this Design Space a Dow fire and explosion index was made and an economic evaluation was carried out. On basis of figure 1 preliminary mass balances were calculated. The following reports listed were made for Design Space 1 and are included as appendices to this report.

- R101 – Feedstock, product, byproduct specifications
- R102 - DOW fire and explosion index
- R103 - Waste and by-product streams
- R104 – Economics
- R105 - European environmental legislation
- R106 - Utilities and auxiliaries
- R107 – Preliminary mass balances
- R108 – Possible use of additives
- R109 - Quality of water

Also a start was made with the Pure Component Properties. The DOW F&EI was calculated in F&EI DS 1.

The main conclusions for these reports are:

- The process shall be operated continuously.
- To reach the product specifications it is necessary to upgrade the Fischer-Tropsch products.
- It's not that viable to sell your diesel just as a cetane booster for poorer diesel. Except if there is a large on location demand for our diesel by another part of the plant.
- As much as possible water from the FT process must be recycled. If the water is pure enough it can maybe be sold as drink- or irrigation water.
- Selling naphtha, LPG, gas-oil and wax as byproducts will depend on the economics for the process.
- CO_2 will probably be discharged into the atmosphere, since there are no stringent environmental guidelines that prohibit the emission. Depending on its purity it may also be sold.
- For NO_x emission limitations were found.
- The auxiliaries and utilities to be used are steam, oxygen, furnace fuel, cooling water/oil and electricity.
- The use of auxiliaries and utilities should be minimized.
- A Dow fire and explosion index of 182 was found. According to the Dow index guide this means there is a severe degree of hazard. This means that safety measurements must be implemented. These results are not very accurate, but we should keep in mind that there is a serious risk of fire. Future analysis of the design will result in more accurate and hopefully lower indices.
- An added value of 37,5 USD/ton NG is possible, with the distribution 25:50:25 for diesel/kerosene/naphtha, based on the input output structure of Design Space 1.
- With the distribution 25:50:25 for diesel/kerosene/naphtha, the maximum weight yield of CH_4 is 89%. In the last two points, natural gas was the only feedstock considered.
- The economical potential of the plant is about 1.0 millions dollars per year, which is very low comparing with the estimated revenue (US$ 65 millions) According to the initial calculations, the process does not seem to be economically viable.
- Diesel additives can be used, but the effect is not very large. For the next design spaces isomerization will be used in first instance to lower the operation regime of the fuels.

1.12 PIQUAR evaluation for DS 1

For each Design Space a PIQUAR analysis was done. In this Design Space the first analysis was carried out at the end of the Design Space. The results can be found in an excel file and are available on disk E104 and will be listed in the final creativity chapter. A quality of 0.53 out of 1 was found. It should be stressed that for some criteria it is difficult to asses points, because they have not been considered yet. The points for which the most quality could be won were; product quality and quantity, safety, low production cost, sustainability and return on investment. These points are listed in order of unquality. The point that worried us the most was the return on investment. The return on investment will be very large (or won't even exist) according to our preliminary calculations. Also safety is a point of consideration, because the Dow fire & explosion limit predicted a severe danger. However, these calculations we're not very accurate, so we can expect some improvement on that field. A positive point was keeping the deadlines and planning. The group is of the opinion that planning is going well so far. Also the group spirit is very good.

1.13 Conclusion

The design such as symbolized in Figure 3 and described in the reports R101 to R109 will propagate to the next Design Space. A number of points for consideration are the water waste stream, the sale of by-products, return on investment and the use of additives on diesel.

1.14 Literature

1. J. Grievink, C.P. Luteijn, K.E. Jap A Joe, S. Birmingham, A framework for conceptual design of process plants, Draft, (2001) PSE-group, faculty of applied sciences, Delft University of technology.
2. Lide D.R., Handbook of Chemistry and Physics, 72nd edition, 1991-1992, CRC Press, Boston, (1992)
3. BP company ltd. (1977)
4. Perry, R.H et al., Handbook of Chemical Engineers, 6th Edition, Mc-Graw-Hill Book co. (1984)
5. William L., Liquefied Petroleum Gas, 2nd revised version, John Wiley& Sons, New York (1982)

Design space 2: Sub-processes

Summary

This report discusses the creation of Design Space 2, the formation of sub-processes. Three sub-processes have been identified. Each process is discussed in a separate report. These reports are included as appendices at the end of the final report:

- Appendix 18: Fischer-Tropsch technology description (R201)
- Appendix 19: Synthesis gas production key technology (R202)
- Appendix 20: Product work-up technology description (R203)
- Appendix 21: Mass balances design space 2 (R204)
- Appendix 22: Dow Fire & Explosion index (R205)
- Appendix 23: Block scheme DS 2 (APP201)

The key-output of this design space is the block scheme in Figure 7. It shows the different sub-processes and their connectivity. Furthermore the interaction through the boundary limits is also depicted.

Contents chapter 4

1.15 Scope of design space 2

In this design space the different sub processes are looked into as well as the links between these sub-processes. The different sub processes are synthesis gas production (syngas production), Fischer-Tropsch Synthesis (FTS) and product workup (Hydrocracking/Separation).

1.15.1 *Battery limits, exchange streams and constraints:*

Each object is defined through battery limits and exchange streams and constraints are mentioned. Apart from individual new constraints, all the constraints mentioned in previous design spaces still apply (DS 0, DS 1). In R204 the overall mass balance of each unit is summarized. These balances give compositions of the ingoing and outgoing streams of the units.

1.15.1.1 *Synthesis gas production*

The synthesis gas production starts with the natural gas (R101 for specifications) entering the boundary limit of the entire plant as specified in DS 1). It ends with syngas of the right composition being pumped to the FTS. This section also supplies a separate hydrogen stream needed for the hydrocracker further downstream. Auxiliaries and utilities are to be specified. This process is constrained by the technologies available for syngas production, the demands posed on the synthesis gas by the FT synthesis sub process and the quality and quantity of hydrogen needed for HC. The wastes of this object are CO_2 (both from the reactions during syngas production as from burner fuel), NO_x, water and possibly soot.

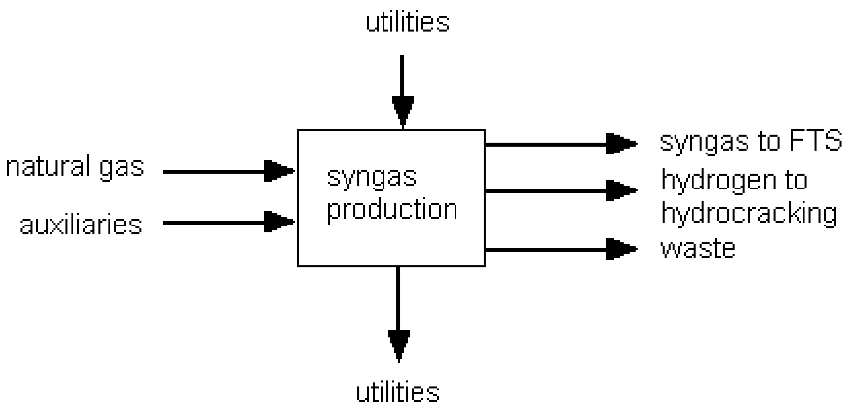

Figure 4: Syngas production

1.15.1.2 Fischer-Tropsch Synthesis

The FTS starts with syngas from the syngas production. It produces long linear hydrocarbons. Auxiliaries and utilities are yet to be specified. A constraint is the fact that FT-technology optimized for wax production should be used. The output of the Fischer-Tropsch reactor is fed to the product workup section. Wastes produced are mainly oxygenates and a very large stream of water (~1 kg water/ kg product).

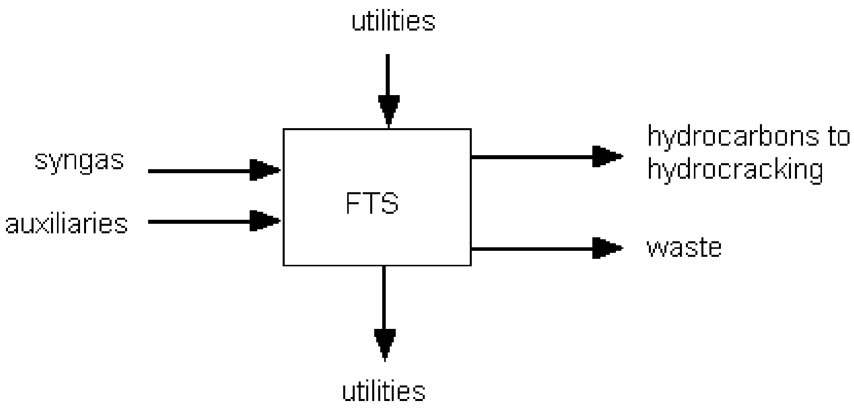

Figure 5: Fischer-Tropsch Synthesis

1.15.1.3 Product workup hydrocracker/separator

In this unit the hydrocracker and separator are combined since they are both responsible for product work-up. The unit is placed behind the FTS and receives hydrocarbons from there. It receives hydrogen from the syngas production. The output stream is ready for distribution. A constraint is the fact that the product should (after cracking and separation) have the right characteristics to be sold as diesel and kerosene (R101).

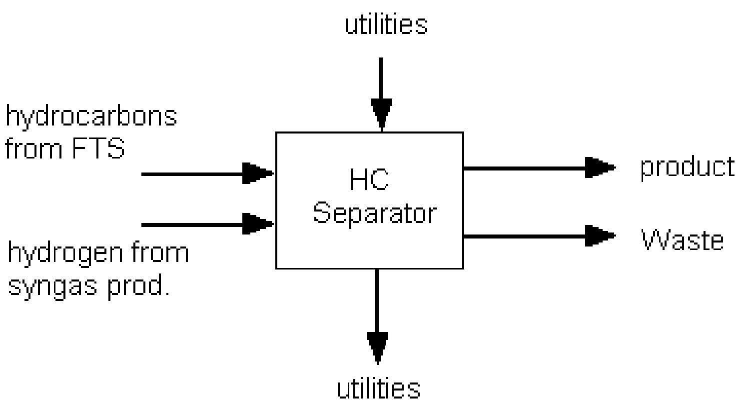

Figure 6: Hydrocracking and separation.

1.15.2 Design decision variables and constraints

- For each of the three techniques a specific technology will be chosen.
- Most other design variables usually treated in DS 2 are set:
  - The way these objects are connected is largely pre-determined by the design assignment. The exact composition and state of the streams between these blocks is decided upon in later design spaces
  - Boundary limits for the sub-processes are already set, only slight variations may occur
  - Because the production rate is quite high the overall process is to be continuous. The sub processes are thus best performed continuous

1.16 Knowledge of objects

The objects for DS 2 have all been set in the Scope of Design:

- The synthesis gas production (syngas production)
- The Fischer-Tropsch Synthesis (FTS)
- The Hydrocracker (HC)

Separation and stream updates are part of the objects. Everyone was assigned an object. Information on different technologies was extended from the former CPD group. Knowledge gathered is described in the following reports, which are included as appendices to the final report:

- Synthesis gas production: R202
- Fischer-Tropsch synthesis: R201
- The product workup section (hydrocracker/separator): R203

1.16.1 Design tools to manipulate objects

The individual sub-processes are evaluated separately to decide the best technology for each block. This is done by looking at different aspects of the performance of each technology.

- Safety
- Economics
- Technology (proven?)
- Product quality and quantity
- Sustainability

During the set-up of the PIQUAR analysis tool in DS 0 (R010) these aspects were found to be of great importance to both designers and principal.

Grades are given for each of these aspects and the importance of the factors is indicated by a multiplication factor. The grades given are from 1-5, five being the best and 1 being the worst. The technology that achieves the highest overall grade (sum of individual grades times weighing factor) is chosen.

Connectivity between the sub-processes is guaranteed by the grades given for product quality and quantity and the grade given for the economics. Quality is low if a block with a certain technology does not comply with the feed specifications set by the subsequent block(s). Connectivity also influences economics, as these will be poor if specifications are not met. This would require extra treatment of product flows and thus extra investment and operating cost. Other factors influence the economics as well.

1.17 Synthesis

Synthesis consisted mainly of finding information on all the different technologies available for the three different sub-processes. After a number of alternatives were gathered and everyone had read the report from the former group, a meeting was called. First the information on the different objects was discussed in the group by means of small presentations from each groupmember. For syngas production seven options were found, for FTS two and for the workup section 3. Again this information can be found in the three earlier mentioned reports.

- Synthesis gas production: R202
- Fischer-Tropsch synthesis: R201
- The product workup section (hydrocracker/separator): R203

After this, each alternative was analyzed and evaluated.

1.18 Analysis and Evaluation

1.18.1 Synthesis gas production

A large number of alternatives were found for the synthesis gas production. As the syngas production is found to comprise up to 60-70 % of process costs (R202), the choice for this technique is the most important of all three sub-processes. Evaluating all these different techniques is done as specified in *knowledge of objects*. The reasoning is explained in the report on the synthesis gas production. The most favorable technique was found to be ATR (Autothermal Reforming), which will be used for further design.

1.18.2 Fisher-Tropsch

Of the two FTS options the HTFT produces mainly light (LPG) products. This meant that because of the constraints in this Design Space only one option (LTFT) remained and further evaluation was not required. The consequence of this invariance in F-T options, further elaborated upon in the previously mentioned R201, is that the other options are dictated by the feed requirements set by the FT unit.

1.18.3 Product Workup

The three workup options differ mostly in the flow sheeting, not much in technique or conditions. For the hydrocracker all techniques rely on high pressure and acid/metal catalysts to force hydrogen into the feed molecules, thus breaking and isomerizing them.

The main difference between the three options is the sensitivity for nitrogen compounds in the feed and the product distribution. Previous sub-processes and the natural gas feedstock determine the amount of nitrogen. It was decided that it is best to try to remove all nitrogen before the HC section.

From the three configurations that were examined the configuration with first the hydrocracking and after that the separation seems the best option for the moment. We are afraid that with the two other configurations (once-through, first separation and then hydrocracking) the product specs for the middle distillates and kerosene are not met.

1.18.4 PIQUAR Evaluation for DS 2

For each design space a PIQUAR analysis was done. In this design space one analysis was carried out at the end of the designing period for DS 2. The results can be found in an excel file and are available on disk [E205]. The PIQUAR analysis showed no improvement in our feeling of quality of the design. The reason for this is that there are still many unknowns. The safety aspect however improved, because the DOW F&EI showed an improvement. The possibility of recycling part of the wastewater is a positive point toward sustainability, but we have no knowledge about the requirements and costs of treating this wastewater before it can be recycled. The only significant change in the quality judgment was noticed for the item “Keeping deadlines and good planning”, due to a delay in the delivery of the DS2 report.

1.18.5 Safety

The safety of the plant is analysed in the report R205. With an index of 149 the syngas unit seems to be the most dangerous unit.

1.19 Results

The block scheme of Figure 7 is the result of this design space. A more detailed block diagram is shown in appendix APP201. The mass streams connected the different blocks are also estimated (R204).
Apart from everything specified above, some overall integration was carried out. The FTS process produces an estimated 1 kg water/ kg product, a very large waste stream. Part of this water could be used in the ATR syngas unit, which uses a certain amount of water as feedstock (this was incorporated in the evaluation process for synthesis gas technology in the criterion sustainability). It is yet to be decided if an oxygen plant is to be installed on location or if oxygen can be acquired from other plants outside battery limits.

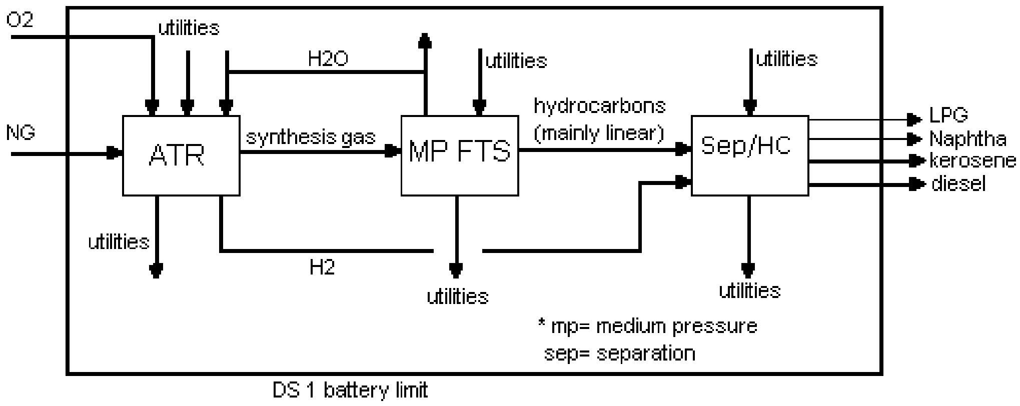

Figure 7: Overall plant block scheme for DS 2.

1.20 Conclusion

The design as it is symbolized in Figure 7 and described in DS 2 reports will propagate to the next design space. A number of points for consideration are the hydrocracker concerning the degree of isomerization and conversion, the oxygen production or purchase, the CO_2 recycle for the syngas production and amount of hydrogen needed for cracking.

1.21 Literature

1. J. Grievink, C.P. Luteijn, K.E. Jap A Joe, S. Birmingham, A framework for conceptual design of process plants, Draft, (2001) PSE-group, faculty of applied sciences, Delft University of technology.

Design space 3: States

Summary

This report discusses the creation of Design Space 3, the description of states (physical and chemical) and the generation of tasks. The tasks that are necessary to convert natural gas into synthetic oil products are presented and described in three reports. These reports are included as appendices. In this design space a more detailed flowsheet is chosen from the four alternatives presented during the basis of design. In order to have a better feeling for the tasks that are necessary a preliminary evaluation of the available hydrogen purification technologies is made. To investigate the effects of the type of Fischer-Tropsch reactor on the tasks and states also an evaluation of the different FT reactors is made, however the precise technology is not chosen yet in this design space. Finally, an evaluation of the thermodynamic equilibrium behavior of the synthesis gas reactions is made and a safety analysis is made. A number of appendices are made that support the contents of this chapter, these are:

- Appendix 24: Blockscheme with mass flows from BOD [APP303]
- Appendix 25: Overview tasks DS3 [APP302]
- Appendix 26: Syngas production states / tasks [R301]
- Appendix 27: FT states / tasks [R302]

- Appendix 28: Product workup states / tasks [R303]
- Appendix 29: Mass balances DS3 [R304]
- Appendix 30: FT reactor evaluation [R305]
- Appendix 31: H_2 separation technology evaluation [R306]
- Appendix 32: Flowsheet selection DS 3 [R307]
- Appendix 33: DOW F&EI DS3 [R308]
- Appendix 34: Syngas thermodynamics [R309]
- Appendix 35: Chosen flowsheet DS3 [R310]

The most important output of this design space is the overview with all the tasks that are necessary to convert natural gas into synthetic oil products [APP302]. During design space 3 the team made a basis of design (BOD) report file and gave a presentation of the BOD. The BOD report file is available as appendix in this report:

- Appendix 36: Basis of design report [BOD]

Contents chapter 5

1.22 Scope of design space 3

In design space 3 the states (physical and chemical) of the streams in the design are described. Design space 3 also concerns the generation of tasks. A task is an operation that effects a change in the physical or chemical state of a material stream (or an amount of material). The states that are most interesting for our design are:

- Chemical identity
- Thermodynamic phase
- Chemical composition of each thermodynamic phase
- Temperature
- Pressure
- Mass (flow rate)

As a starting point for the generation of tasks the blockscheme from DS 2 is taken as a starting point [APP201]. In this blockscheme a number of objects can be described. The objects in this design space are the locations where at least one of the states is altered. The objects themselves are considered as a black box, but the objects have to perform a specific task. For every task feasible targets must be set. For these tasks also the means to accomplish this task in terms of driving forces must be identified. Finally, it is important that the possible side effects of each task are identified.

1.22.1 Battery limits, exchange streams, constraints:

The battery limit of each object is the in- and outgoing stream together with the black box that represents the task that needs to be done. For every task the exchange streams are described with a mass balance and these balances are used to generate an overview of all the mass balances of the design. In some cases the key technology that has to be used is a constraint. In design space 2 already some key technologies are chosen in order to prevent taking too much variables to design space 3. When a specific task is described this key technology has to be taken into account. Off course all the other constraints from the previous design spaces [DS0, DS 1 and DS 2] still apply.

1.22.2 Design decision variables

The decision variables of this design space are:

- Function of tasks
- Boundaries of tasks
- Ports (mass or energy)
- Connectivity of tasks
- Technology to be used (if necessary).
- Connecting streams and their specifications (states)
- Duties for tasks
- Throughput

The design decision variables of the objects are described in three reports:

- Syngas production tasks [R301]
- Fischer-Tropsch technology tasks [R302]
- Product workup tasks [R303]

The connection of the objects has to be chosen by means of a rough economic estimation of the four flowsheet alternatives that are presented during the basis of design [BOD]. The main decision variables during this selection are the place of the hydrogen recovery unit and the carbon dioxide recovery unit.

The design will be performed by a team of 3 designers and has to be completed on 10-06-2003.

1.23 Knowledge of objects

Knowledge is gathered on the mayor units that are involved in the process (syngas production, Fischer Tropsch unit and product upgrading). This knowledge concerns mostly operating conditions of the different units.

The objects of this design space are described in the scope of design and are shown in appendix 302 [APP302]. The knowledge that is available and gathered is summarized in the following reports:

- Syngas production tasks [R301]
- Fischer-Tropsch technology tasks [R302]
- Product workup tasks [R303]
- General mass balances from BOD [R304]

In order to get a feeling for the equilibrium behavior of the reactions that play an important role in the synthesis gas production, a report is made where the influence of the various operating conditions on the equilibrium is investigated. This report is available as an appendix [R309]. Moreover information is gathered about the possibilities for the technology that can be used to accomplish certain tasks. Although equipment selection and/or technology selection is not a topic for design space 3, the team decided to do a preliminary study about technologies that can be used to accomplish certain tasks. This will give more insight on the type of tasks that are necessary to change a certain state. These studies are made for the hydrogen recovery (necessary before and after the hydrocracker) and for the Fischer-Tropsch reactor and are available as appendices:

- Hydrogen separation technologies [R306]
- Fischer-Tropsch reactor evaluation [R305]

1.23.1 Design tools to manipulate objects

As in DS2, there are design tools, which influence the choice of a certain task. These design tools also play an important role in the placement sequence of these tasks. In this design space the criteria from the PIQUAR tool are also used [R010] as criteria to make a choice and to evaluate the design.

In this design space a choice should be made on which tasks should be performed to finally satisfy the product and production requirements of the client. Not only which tasks should be performed is important, but also the order in which they should be placed.

The choice of tasks in each of the three units and the order in which they are placed is a trade of between:

- Price of the equipment used for the tasks
- The utility necessary
- Efficiency of placing the tasks behind its predecessor.
- How safe is the operation of this task.
- Operability

So a combination is made out of the different factors and from this with the help of rough economic estimation procedures an optimal scheme of tasks is chosen.

1.24 Synthesis

The synthesis phase as stated earlier, is on the choice of tasks and the placement of these tasks in a certain order. With the knowledge of the approximate operating conditions, the tasks that need to be performed to convert natural gas into the desired product stream are generated.

The mayor tasks in design space 3 involve tasks that are related to:

- The syngas unit
- The Fischer –Tropsch unit
- The product work up (includes the hydrocracker and the distillation)
- Water recovery

- Hydrogen recovery
- Carbon dioxide recovery
- Separators

The order of all the tasks is dependant on the general flowsheet. The chosen flow sheet is discussed in appendix 32: flow sheet selection [R307]. The design alternatives are generated by varying the hydrogen recovery unit for the hydrocracker and by varying the carbon dioxide recovery unit. The flowsheet configuration that is chosen is the first flowsheet that is proposed during the BOD and is available in appendix 35 [R310].

According to the selected flowsheet tasks are synthesized for each section in a report:

- Syngas production states [R301]
- Fischer-Tropsch states [R302]
- Product work up states [R303]

From all these states in the different sections a graph is made, which shows all the tasks of the entire process [APP302]. A general mass balance is described in R304 and APP303.

1.25 Analysis and Evaluation

The choice of process flow sheet with its accompanying tasks was analyzed mostly by judging the process economics. Furthermore, by taking into account the effects of the unit 'tasks' on each other. It turned out that placing the hydrogen recovery unit and the carbon dioxide before the Fischer-Tropsch reactor has the highest economic potential. This result was obtained by rough economic estimations. It turned out that the compression costs outweighed the material costs. However it should be noticed that a lot of factors are not taken into account during the evaluation of the economics that could have an important effect, these are for example:

- The utilities, the wastes and the quality of the CO_2 separation if a separate CO_2 separation unit is used.
- The implementation of a synthesis gas recycle to the FT reactor
- The influence of CO_2 in the FT reactor on the kinetics

An overview of the all the tasks that are necessary to convert natural gas into synthetic oil products is given in appendix 25 [APP302].

For a more detail reasoning behind the choice of the flow sheet and the description of the accompanying tasks reference is made to:

- Flow sheet selection [R307].
- Chosen flowsheet DS3 [R310]
- Syngas production states [R301]
- Fischer-Tropsch states [R302]
- Product work up states [R303]

1.25.1 *PIQUAR Evaluation for DS 3*

For each design space a PIQUAR analysis was done. Also in this design space an analysis was carried out at the end of the designing period. The results can be found in an excel file and are available in appendix 6.
For the this design stage the average piquar number increased, partly due to the fact that more knowledge is gathered on the different criteria. The mayor increases were sustainability, operability and innovative design. E.g. the sustainability generally scored higher because now more was known about what would be done with the waste streams, the amounts that would be recycled etc. So a better quantitative grasp was achieved on the processes sustainability. The plant is now considered to be better operable, primarily because of the use of a CO2 recycle. In this design space, because more room is available, we used more of our own innovation especially for the implementation of the recycle streams. The most noticeable decreases were keeping deadlines and the use of creativity and process tools.
Due to time shortage and a misjudgment in the planning, the deadline for the BOD was not kept. Another consequence of the time shortage was that the use of the AAA was neglected.

1.25.2 *Safety*

The safety of the plant is analysed by determining the DOW Fire & Explosion index, this result is available in appendix 33 [R305]. The safety of the plant does not deviate that much from the analyses from DS2. Although with an index of 147 the syngas unit safety slightly increased. But all the units still maintained the same classifications and the syngas unit still is the most dangerous process unit.

1.26 Results

From synthesis of the known objects an optimal configuration was chosen. All the proposed tasks in the process are identified in the order in which they will be used. [APP302].

Finally with this configuration after each task we can define stream flows and the change in:

- Chemical identity
- Thermodynamic phase
- Chemical composition of each thermodynamic phase
- Temperature
- Pressure
- Mass flow rate

1.27 Conclusion

From the flow sheet selection the basis is now set on which type of flow sheet will be used further during the design. With this choice and the tasks assigned to the different units in this flow sheet we can move up to the next design space and have a deeper look into the chosen tasks “units”. During this next design space a more detailed mass balance will be developed according to the chosen flowsheet.

A point for consideration is the hydrocracker concerning the method of isomerization (extra isomerization reactor or one large hydrocracker). Also it is a good consideration to investigate how we can shift the product distribution of FT unit more to kerosene and diesel because still too much naphtha is produced. Furthermore at the start of design space 4 a catalyst should be chosen for the FT reactor, because the type of catalyst influences the rates of change that are described in DS4.

Also at the start of DS4 a meeting will be held with the creativity coach to review the best possibilities of integrating the different tasks and possibly improve the chosen flowsheet.

1.28 Literature

1. J. Grievink et.al., 2001, A framework for conceptual design of process plants.

Design space 4: unit operations

Summary

This report discusses the creation of Design Space 4. In this design space the rates of change (heat and mass transfer) are the important factors. Also the contacting patterns are described and designed in this design space. In this design space the three mayor sections were again the syngas production section, the FT reactor section and the product workup section. The different units and the tasks for these units, the rates of change of heat and mass, were produced in a number reports. The reports that support this chapter are available as appendices:

- Appendix 37: Product isomerization configuration selection [R401]
- Appendix 38: FT catalyst selection [R402]
- Appendix 39: Rates of changes syngas production [R404]
- Appendix 40: Rates of change FT section [R408]
- Appendix 41: Rates of change distillation columns [R405]
- Appendix 42: Rates of change hydrocracker [R406]
- Appendix 43: Rates of change isomerization reactor [R407]
- Appendix 44: Flowsheet upgrade selection [R409]
- Appendix 45: DOW fire & explosion index [R410]
- Appendix 46: Aspen model results [R411]
- Appendix 47: Aspen report file

The process is simulated with AspenPlus11 from which a stream table is obtained that contains all the mass balances and heat balances of each section. The most important results of this design space are a more detailed flowsheet and all the heat and mass balances.

Contents chapter 6

1.29 Scope of design space 4

This design space addresses the unit-operations, which compromises one or more tasks that are carried out simultaneously in the same spatial environment. Unit-operations deal primarily with rates of changes (e.g. mass transfer, heat transfer) in an abstract geometrical subspace. Therefore, kinetics and transfer rates are part of the component mass- and energy balances in this design space. For conditions close to thermodynamic equilibrium (e.g. the ATR reactor) the compositions and rates can be calculated with thermodynamic equilibrium calculations. For conditions far from thermodynamic equilibrium (e.g. the Fischer-Tropsch reactor) transfer rates are calculated with kinetic relations. Heat duties are also considered in unit-operations, as well as contacting agents and contacting patterns between phases. The targets set in design space 3 are taken as a starting point for designing e.g. sufficient residence time, contacting areas, and theoretical contacting stages within the unit operation. This design space can be divided in five subspaces:

- *Conversion and recycle structure*: Topics are for example the conversion of methane to syngas, the conversion of syngas to hydrocarbons or the conversion of heavy waxes to synthetic fuels. Also the rates of changes of the recycle structures are calculated (CO_2 recycle and syngas recycle are important recycles)
- *Separation*: Topics are for example the separation of the final product into hydrocarbons in the desired range or the separation of carbon dioxide.
- *Product synthesis*: An important topic relating to this subspace is for example the product isomerization.
- *Feedstock conditioning and product work*-up: most of the topics relating to this subspace are outside our battery limit (e.g. compression and storage of LPG)
- *Process integration*: This subspace is meant for combining several unit-operations into one lumped unit-operation.

1.29.1 *Battery limits, exchange streams, constraints:*

The battery limits of the units are the reactions taking place in the units and the effect of the reactions on composition of the streams and the temperature. The rates of mass transfer and heat transfer are important for a good overall control of the process. For every unit the exchange streams are described with mass and heat balances with transfer rates and these balances are used to generate an overview of all the mass and heat balances of the design. The contacting agents and the patterns are also set in this design space. The process variables for process control must be selected. The controlled variables are selected in such a way that targets that are set are met. For the controlled variables manipulated variables must be available in order to keep the controlled variables at the desired value. Additionally the design must be able to handle disturbances.

An important constraint in this design space is the demand that the process is controllable. In some cases the key technology that has to be used is also a constraint. In design space 2 and 3 already some key technologies are chosen in order to prevent taking too much variables to the following design spaces. Off course all the other constraints from the previous design spaces [DS0, DS 1, DS 2 and DS3] still apply.

1.29.2 *Design decision variables*

The decision variables of this design space are:

- Function of units
- Boundaries of tasks

- Ports (mass or energy)
- Connectivity of units
- Technology to be used (if necessary).
- Connecting streams and their specifications (states)
- Mass transfer rates
- Heat transfer rates
- The relative cost of the units
- Contacting patterns

The alternatives for the design decision variables of the objects are described in five reports, which are included as appendices:

- The most important design decision variables of appendix 39: Rates of change Syngas section [R404] are:
  - Catalyst selection
  - Water recovery operating conditions
  - CO_2 recovery operating conditions / contacting patterns

- The most important design decision variables of appendix 40: Rates of change Fischer-Tropsch section [R408] are:
  - Catalyst selection
  - Contacting patterns
  - Operating conditions

- The most important design decision variables of appendix 41: Rates of change distillation [R405] are:
  - Recovery
  - Number of contacting stages
  - Reflux ratios
  - Contacting patterns
  - Operating conditions
  - Feed conditions
  - Thermodynamic model
  - Reboiler / condenser duties
  - Number and sequence of columns

- The most important design decision variables of appendix 42: Rates of change hydrocracker [R406] are:
  - Catalyst selection
  - Operating conditions
  - Contacting pattern
  - Modeling (a choice is made between a typical known product distribution or modeling with approximate kinetics)
  - Cooling duty / contacting pattern
  - Hydrogen recycle method and operating conditions

- The most important design decision variables of appendix 43: Rates of change isomerization section [R407] are:
  - Catalyst selection
  - Operating conditions
  - Contacting patterns
  - Cooling duty / contacting pattern

The total process was modeled in AspenPlus to incorporate the different units with each other and control the process with the right operating conditions. With this model all the heat and mass balances are incorporated. This model gives the team also more insight in the effect of linking the different units.

The design will be performed by a team of 3 designers and has to be completed on 10-06-2003.

1.30 Knowledge of objects

The objects of this design are described in the scope of design. The knowledge that is gathered on the different unit operations is than further specified in the previously mentioned appendices from the three different sections. More information was gathered in order to synthesize alternatives for the design decision variables. The knowledge is described in the previous mentioned appendices. The most important knowledge that is generated for this design space is related to:

- ATR catalyst possibilities:
  - A Ni δ-alumina catalyst is suitable for the steam reforming part in the ATR

- FT catalyst possibilities:
  - An Iron catalyst can be used
  - A cobalt catalyst is also suitable
  - A comparison is made between the two catalysts and cobalt is chosen as the preferred catalyst

- Hydrocracking catalyst possibilities:
  - Many catalyst are available for hydrocracking
  - A NiMo-γ-alumina is chosen for the hydrocracker

- Isomerization catalyst possibilities:
  - Four different catalyst are described
  - A SAPO-11 zeolite catalyst is chosen with Pd

- The possibilities for a selective CO_2 separation

  - An absorption unit turned out to be more expensive and larger than was expected in design space 3.

- Fischer-Tropsch reaction kinetics:
  - It is decided to calculate the rates of changes with the earlier determined product distribution. The kinetics of the Fischer-Tropsch reaction is used in design space 6 to size the equipment.

- Influence of contacting pattern on Fischer-Tropsch reactor
  - The catalyst and reactants are contacted in a slurry reactor

- Hydrocracking product distributions and kinetics
  - A typical product distribution from industry is described
  - A kinetic model based on the conversion of heavy feedstocks is evaluated
  - A kinetic model of model components (C_8, C_{12} and C_{16}) is evaluated
  - The known product distribution is determined to be the best way of modeling the hydrocracker

- Hydrogen separation for hydrocracker recycle
  - A sensitivity analysis showed that a low temperature gas/liquid separator can be used

- Isomerization product distribution and operating conditions:
  - The degree of product isomerization is large enough and the degree of cracking is acceptable

- Short-cut calculations for crude distillations
  - The DSTWU short-cut method, which is available in AspenPlus11.1, is used for the wax/middle distillate separation
  - The SCFrac short-cut method, which is available in AspenPlus11.1, is used for the fractionator modeling

Some more information is gathered on different subject that made the team reevaluate the flowsheet configuration, these were:

- The modeling of CO2 absorber
- The syngas separation and recycle
- The product streams from the Fischer-Tropsch reactor.
- The products from the isomerization reactor
- The preferred technology for the hydrogen separation after the hydrocracker

With the new additional information that was the overall flow sheet of the process was further upgraded. A few options were again evaluated and the final choice and reasoning is given in the report on the reevaluated flow sheet selection [R409]. The knowledge that is obtained about these subjects is further explained in the corresponding appendices.

1.30.1 Design tools to manipulate objects

As in the previous design spaces there are design tools, which influence the choices that were made. In this design space these tools influence the choice of a certain unit operation and or process condition(s) above another. In this design space the criteria from the PIQUAR tool are also used [R010] as criteria to make a choice and to evaluate the design.

As in the previous design space the chosen units and the operating conditions are also steered by the requirements of the client. The aim is to reach the production capacity, as efficiently and effectively as possible also here the same trade offs should be made between:

- Economics
- Product quality and quantity
- Safety
- Controllability and operability of the process
- Sustainability

With the help of these PIQUAR factors the optimal choice in flow sheet for effective heat and mass transfer is chosen.

In this design space a new design tool that is frequently used is the steady state flowsheet software AspenPlus11.1®. This tool is especially useful in linking the different units and getting a feel of the operating conditions and heat effects of the flowsheet.

1.31 Synthesis

In this design space the synthesis phase consists of specifying the units that will be used, the conditions in the units, the mode of operation so the mass and the heat transfer in the units, finally the entire process can be calculated and brought up to the requirements of the client. The choice of these units is based on most effectively incorporating the tasks that need to be performed in the previous design space.

With the knowledge gathered on the mass transfer rates and the heat transfer rates, preferred recoveries etc. units were chosen to optimally be able to perform the tasks. The main tool that was used to accomplish this task was AspenPlus. The knowledge that was gathered during the previous design cycle made the team reconsider some of the flowsheet configurations. New flowsheet alternatives were synthesized during this design space. This synthesis is described in two appendices:

- R401 – Product isomerization:
    - The team investigated the possibility of using an isomerization reactor to reach the required cloud and pour point for diesel and the required freeze point for kerosene. Three options are synthesized. The difference in the options is the use of an isomerization reactor and the place of the separation unit.

- R409 – Flowsheet upgrade selection
    - Three flowsheet configurations were synthesized that matches the latest available knowledge best. The configurations differ in the separation sequence and the placing of the hydrocracker and the isomerization reactor. The locations of the recycles are also varied for the different options. After the evaluation a fourth alternative is added that is supposed to be an improvement of the best option of the first alternatives. For more details about the synthesized flowsheet configurations reference is made to appendix 44 [R409].

With the specification and the units and its capabilities the process is then completely modeled in ASPEN to produce the required production capacity. The main units that were connected and modeled in AspenPlus were:

- A unit for syngas production (ATR)
- A water recovery
- A unit for syngas conversion (FT- reactor)
- The hydrocracker
- The isomerization reactor
- The distillation column(s)
- Flash vessels
- Hydrogen recovery
- Separators

The choice and synthesis of units and their operating conditions are explained in the earlier mentioned appendices:

- Rates of change Syngas section [R404]
- Rates of change distillation [R405]
- Rates of change hydrocracker [R406]

- Rates of change isomerization section [R407]
- Rates of change Fischer-Tropsch section [R408]

The results of the complete model, which is synthesized with AspenPlus is presented in an appendix:

- Aspen model results [R411]

The document with the stream table gives an overview of all the streams with their properties. This document contains all the mass and heat balances as well as the thermodynamic state of each stream. The flowsheet drawing gives an overview of the connectivity of the streams and blocks. The reasoning behind this connectivity is mainly explained in the documents about flowsheet configurations during design space 3 and 4 [R307, R401 and R409].

1.32 Analysis and Evaluation

The choice of process flow sheet with its accompanying units was analyzed by judging PIQUAR quality factors of the process, with new knowledge that was gathered about separations and the isomerization of the product. Furthermore the effects of the units on each other are important. These effects are made clear with the AspenPlus simulation. The feasibility of the entire process is investigated with the model of the process. The most important changes or new elements that were added during this design space were:

- A combined carbon dioxide and syngas recycle
- One separation for carbon dioxide, syngas and products
- An isomerization reactor before the final separation
- A flash vessel for the hydrogen recovery after the hydrocracker
- A preflash column before the final separation

The properties and connectivity of all the streams are reported in appendix 46 [R411]. The most important yields of the complete model of the process are presented in Table 3. The yield of the feed over the utilities is calculated in a later design space, because the heat integration is the topic for design space 5.

Table 3: Main yields of the process

Property	Value	Units
Feed/product*	1.57	kg NG/kg P
Naphtha selectivity	0.15	kg Naphtha/kg NG
Kerosene selectivity	0.24	kg kerosene/kg NG

Diesel selectivity	0.25	kg Diesel/kg NG
CO_2/Feed	0.68	kg CO_2/kg NG
H_2O/Feed	1.25	kg H_2O/kg NG
Wax//Feed	$2.23 \cdot 10^{-3}$	kg wax/kg NG
process chemicals**/Feed	1.18	kg O_2/kg NG
Product/syngas	0.35	kg P/kg SG
Syngas out/syngas produced	$7.9 \cdot 10^{-2}$	kg SG/kg SG

* Naphtha, kerosene and diesel
** O_2

With Table 3 it is possible to compare the designed process with existing processes. The table also shows that the total conversion of syngas is 92% (yield of syngas out via purge vs the amount of syngas that is produced).

The overall heat and mass balance of the process is presented in Table 4.

Table 4: Overall heat and mass balance

	Mass in [kt/a]	**Mass out [kt/a]**
Natural gas	787.0	
Oxygen in ATR	926.2	
Oxygen in burner	296.2	
Water/steam	23.2	985.0
CO_2		536.0
Naphtha		117.8
Kerosene		187.3
Diesel		196.0
Wax		1.8
H_2 purge		1.5
N_2 out		7.1
Total	2032.6	2032.5
	Enthalpy in [MMBtu/hr]	**Enthalpy out [MMBtu/hr]**
	-469.4	-2155.3

The values from the Table 3 and Table 4 are taken from the report file with the stream table [R411].

1.32.1 Economic potential

Now the streams are known in more detail the economic potential can be recalculated. The economic potential calculation is presented in Table 5.

Table 5: Economic potential calculation

Component	In / out	Mass flow [kt/a]	Price [USD/t]	Value [10^3 USD]
Natural gas	IN	787	92.5	-72,798
Oxygen	IN	926.2	27.0	-25,007
Steam (fract.)	IN	23.2	1.30	0
Water	OUT	985	0	0
Naphtha	OUT	117	130	15,210
Kerosene	OUT	188	135	25,380
Diesel	OUT	196	120	23,520
Wax	OUT	1.8	0	0
			Total	-33,000

If we compare the economical potential of design space 4 with the latest economical potential calculation (appendix 11), it is clear that the economical potential has decreased. The main cause for this is a higher selectivity for diesel and a lower selectivity for kerosene than expected in design 1.

1.32.2 *PIQUAR Evaluation for DS 4*

The PIQUAR evaluation for design space 4 shows some improvement in the quality of the project. The quality factor increased from 5.8 to 7.0. For each design space a PIQUAR analysis was done. The main improvements were achieved in the economical performance of the plant and in the product quality and quantity. There little or no improvement in the use of project tools and in aspects as communication and documentation. These factors are very important and should be improved in the following phases of the project. More detailed information about the PIQUAR evaluation for DS4 can be found in appendix 6: PIQUAR

1.32.3 *Safety*

The safety of the plant is analysed in the report for the F&EI [R410]. The safety of the plant as a whole decreased a bit because the exact amount of products, reactants are now final to obtain the production capacity. The value of the FT reactor changed slightly, but the others were similar to that of DS3. The classification of the FT changed to moderate, while that of the other units stayed the same. The syngas unit still proposes the largest degree of hazard.

1.33 Results

The object of study of this design space is the rate of change (heat and mass transfer) of the most important units. Also the contacting patterns are described and designed in this design space. The results for each unit are available in the following documents:

- Rates of change Syngas section [R404]
- Rates of change distillation [R405]
- Rates of change hydrocracker [R406]
- Rates of change isomerization section [R407]
- Rates of change Fischer-Tropsch section [R408]

A flowsheet was made based on these rates of change. A process simulation was performed using ASPEN PLUS and the results are available in appendix 46 and appendix 47.

1.34 Conclusion

In this design space the final flowsheet configuration is fixed except for the heat exchange network, which will be the subject for the next design space. In this design space all the heat and mass balances are determined and available in the appendices. In the next design spaces choices will be made about the way the mass transfers are accomplished (equipment design, design space 6) and the heat transfer rates are accomplished (heat integration, design space 5).

During design space 4 some decisions that were taken in earlier design spaces were revised, for example:

- The location and the method of the CO_2 recovery
- The implementation and location of a isomerization reactor
- The separation sequence of the product streams

These changes would require the team to move back to the beginning of design space 3, because the tasks that are necessary to accomplish the conversion of natural gas into synthetic fuels products are changed. Especially the sequence of the tasks is changed. The team considered the consequences of going back to design space 3 and concluded that going back to design space 3 and changing the contents of design space 3 would leave hardly any time for design space 5,6 and 7. The priority is set to finishing design space 5,6 and 7. It is of because this latter reason that the team decided that the current design could propagate to design space 5.

1.35 Literature

1. J. Grievink et.al., 2001, A framework for conceptual design of process plants.

Design space 5: Process integration

Summary

In this design stage, the heat exchanger network was designed in order to make a better use of the heat produced during the process. The overall process is exothermic and the heat produced by the Fischer-Tropsch reactor and by cooling down the ATR effluent can be used to heat up other process streams. In this heat integration process, only the large heat streams were taken into consideration. Special attention was paid to the controllability safety of the process and not only to the thermodynamic optimization of the heat integration. For this design space a number of appendices are available that support the contents of this chapter, these are:

- Appendix 48: Summary of Streams (E501)
- Appendix 49: Final ASPEN model with Stream Table (E503)
- Appendix 50: HEN (R501)
- Appendix 51: Heat Exchangers (R502)
- Appendix 65: final flowsheet and stream table (E502+ P501)

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1.36 Scope of design space 5

Design space 5 refers to plant-wide heat and solvent integration. The different unit operations involved in the process were treated in design space 4. Now, in design space 5, these unit operations should be integrated in such a way that the process will consume less energy and produce less by-products. At the same time, the process should remain controllable and safe. Economical aspects must be also kept in mind while performing a process-wide heat or solvent integration. This process makes no use of solvents and only heat integration was carried out in design space 5.

1.36.1 Battery limits, exchange streams, constraints:

At first all the constraints from the previous design spaces [DS0, DS 1, DS 2, DS3 and DS4] apply for DS5.

The tasks of design space 5 are limited to the connectivity of streams from DS4. The most important constraints to this connectivity are

- Amount of heat available per stream
- Temperature at which heat is available
- Controllability of the system
- Process safety
- Economic feasibility of heat integration

The most important exchange streams are

- Cooling water

- High-, medium- and low pressure stream (consumed and produced by the process)

In the case of production of surplus steam, this steam could be used outside the Fischer-Tropsch plant, but this is outside the battery limits of the process. Steam produced and consumed in this process will be delivered by pipe following the specifications given in R101.

1.36.2 Design decision variables

The decision variables in this design space are:

- Connectivity between the streams
- Contacting pattern (co-current, countercurrent, multiple loops)
- Heat exchanging area
- The materials of construction (e.g. corrosion resistant, relatively cheap)

The connectivity between the different heat flows and the heat exchanger network is explained in R501.

The plant design contains more than 15 heat exchangers. Because of time constraint, only 5 heat exchangers could be sized. All other heat exchangers were scaled based on the heat duty, temperature gradient and type of stream (liquid, vapor, organic, water etc). The results for the dimensioning of the heat exchangers can be found in R503.

1.37 Knowledge of objects

1.37.1 Design tools to manipulate objects

In this design space we have specially made use of two design tools:

- ASPEN flowsheet simulation
- Pinch Technology

The flowsheet simulation program was used to calculate the heat streams and estimate the heat capacity of each stream. With this data is was possible to perform heat integration using the pinch temperature approach.

The team performed brainstorm sessions in order to come with ideas for different combination of heat streams. During these sessions, we have made use of visualization, using large drawings of the process flow sheet. We have also used different “hats” during this session in order to analyze and evaluate the different possibilities for combining heat streams.

1.38 Synthesis

The objective of this design space is to integrate heat streams within the plant in order to make optimal use of the heat produced in the process. This integration was done by means of the pinch technology, using the heat streams calculated with an ASPEN flowsheet. After designing a heat exchanger network, some of the heat exchangers were dimensioned and the contacting pattern between the heat streams is defined. The results can be found in the reports mentioned above. The most important feature of the heat integration process is the use of the effluent from the ATR reactor to heat up the reactor feed.

1.39 Analyses and evaluation

The complete heat integration process is a complex work that requires good knowledge of the thermodynamic properties of the streams and involves many other aspects as safety, economics etc. The design of 18 heat exchangers is also a time consuming task. Because of the time constraint, the group has tried to integrate the most important heat streams within the plant, but this subject should be further developed in the future in order to make optimal use of all heat streams.

Also for this design space we have made use of PIQUAR to evaluate the quality of the design.

1.40 Piquar evaluation

The piquar evaluation shows very little improvement comparing to DS4. The total quality factor increased from 0.70 to 0.71. An important improvement in DS5 was the use of creativity tools and the cost of production. In DS5 we came to the conclusion that the process produces a large amount of surplus steam (medium pressure). This steam can be used in other plants in the neighborhood or it can be used to produce electricity.

1.41 Results

The ASPEN model from DS4 was changed to include some of the heat exchangers. The model can be found under the filename DS6 final flowsheet_with HEs.apw. The stream table of this model is on E503. The net heat consumption of the process is about –440 MW (the process is exothermic). To have an idea about the amount of surplus steam produced by the process, we took into account only the steam produced by the FT reactor, which represents major fraction of the total steam production. The steam produced by the FT reactor is then used to run the compressors and is also used in the strippers of the distillation columns. The amount of steam that remains could be exported. This assumption is based on the fact that the main ATR effluent already provides the heat necessary for some of the main cold streams and that certain minor hot streams could eventually be used to heat up other minor cold streams.

The ASPEN model does not contain the complete HEN. The final flowsheet that contains the heat exchanger network can be found in appendix 46: Final flowsheet. This flowsheet contains also a simple control structure, which was designed later in design space 7. This is the flowsheet that must be used as reference for the project.

1.42 Conclusions

Heat integration is a very important part of the process. It depends on various aspects and is a time consuming task. The work done here gives just an idea of the possibility of using combining certain heat streams in order to diminish the use of utilities in the process. In a further stage of the project, more detailed heat integration may be desirable. The heat exchangers should also be discussed and designed with a higher level of details.

1.43 Literature

1. J. Grievink et.al., 2001, A framework for conceptual design of process plants.
2. J.M. Douglas, Conceptual design of chemical processes, McGraw-Hill, Boston, 1988

Design space 6: Equipment design

Summary

In this design space the sizing of a selection of equipment is done. The idea is to get a global idea of what the geometry (size, shape) of that certain equipment is. The sizing of the equipment is produced in a number of reports. Not all of the units present in the flow sheet are sized, a few units are chosen that are believed to have a large contribution to the equipment cost. The units that are considered for sizing are the mayor units, the ATR, the FT slurry reactor, the distillation columns, and the hydrocracker and isomerization reactor. Further a few other units, which are also believed to have a large contribution to the equipment costs such as, compressors, condensers (evaporators) and vapor/liquid separators. Due to lack of time, the few of the smaller units with multiple occurrences in the flow sheet are not all calculated. A few of them are just scaled by a certain factor. With the knowledge about the different equipment dimensions, the equipment costs of the units can be determined. Finally the economic evaluation of the process can be done. A number of appendices are generated that support this chapter, these are:

- Appendix 52: Equipment design FT reactor [R601]
- Appendix 53: Equipment design ATR [R602]
- Appendix 54: Equipment design vapor/liquid separator [R603]
- Appendix 55: Equipment design distillation columns [R604]
- Appendix 56: Equipment design compressors & pumps [R605]
- Appendix 57: Equipment design hydrocracker [R606]
- Appendix 58: Equipment design isomerization reactor [R607]
- Appendix 59: Equipment design heat exchangers [R610]
- Appendix 60: Economic evaluation [R608]
- Appendix 61: DOW fire & explosion index DS 6 [R609]
- Appendix 62: Equipment specifications sheets [APP601]

The most important output of this design space are the equipment specifications sheets, which summarizes the results of the equipment design.

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1.44 Scope of design space 6

In design space six the focus is on the geometry, the shape and the technical details of the equipments presents in the design. For a few of the units that will be sized there are usually a few different types possible. With the knowledge of the process conditions and by taking into account the factors a suitable type of unit can be chosen. With the help of the properties of that certain type and the throughputs the size of the unit can be calculated. The sizing of the equipment is then further used to determine the economic strength of the process.

1.44.1 Battery limits, exchange streams, constraints:

The battery limits for this design space are the sizing of a selection of few units from the design. The mayor units such as the ATR, the FT reactor, the distillation columns, the hydrocracker and the isomerization are sized to a certain degree of detail while the smaller units such as pumps and compressors etc are just modeled in AspenPlus. The most important thing to know about these pieces of equipment is the duty of the equipment, because they contribute significant to the economical result. For the latter the results from AspenPlus such as the work requirements are just taken to have an overview of the “sizes” of these equipments. The piping of the design was also left out of the battery limit of this design space. The membrane separators present in the process (to separate hydrogen from syngas and catalyst from the Fischer-Tropsch reactor) shall also not be designed due to time constraint. In the economic calculation the equipment cost for these separators are estimated by scaling the equipment with equipment in the same section as the membrane is placed.

All the constraints from the previous design spaces [DS0, DS 1, DS 2, DS3, DS4 and DS5] apply for DS6. Additional targets and constraints are:

- Throughputs and operating conditions the units are required to handle.
- Equipment integrity and maintainability
- Physical space the equipment is allowed to occupy
- All streams and specification form DS5
- Controllability
- The connectivity of the unit operations for control
- The investment cost targets and a refined economic potential

1.44.2 Design decision variables

The decision variables are for efficient and sustainable processing of the fixed throughputs. The decision variables in this design space are:

- Type, geometry and number of equipments to be used
- The ports (mass, energy)
- The connectivity of the equipment
- The materials of construction (e.g. corrosion resistant, relatively cheap)
- Size of the equipment
- Size of the equipment internals
- Phase ratio's
- The residence time or contacting times in the different units

In the sizing of the equipments, calculations are done to get a feeling of the size range of the different equipments. For the smaller units, from which there are more present in the process and which have a significant contribution to the costs, only one of them is sized and the others are sized by scaling the capacity. From the equipment design, equipment data sheets are developed to specify the process units in detail [App601].

1.45 Knowledge of objects

Before the sizing of the equipment can take place, knowledge is gathered on the objects mentioned in the scope of design. All the decisions made in choosing a certain type of unit were based on the knowledge of the specification of the process that needs to be performed and the capability of that type of unit to operate at those conditions. With this knowledge and the knowledge on the units the equipment can be sized. The knowledge gathered on the units, the streams and the process conditions is presented in:

- Appendix 46: Aspen model results [R411] for process conditions, throughputs and heat duties.
- Chapter 6: The units operations for mass and heat transfer rates [DS4].
- Chapter 7: Heat integration [DS5].

With the results of the sizing of the units, the economics of this process can be further calculated, with the help of cost assessment of the types of units used. The most important knowledge gathered for the economic calculations are estimations for certain types of equipment that are available in literature [2][3].

More specific information that is gathered during this design space is described in more detail in the previous mentioned appendices, they mainly concern:

- Hydrogen attack on metals
  - Due to the nature of our process hydrogen is present in many locations of the plant. It is known from literature [2][4] that at elevated temperatures and significant hydrogen partial pressure, hydrogen will penetrate carbon steel, reacting with the carbon in the steel to form methane. The pressure generated causes a loss of ductility (hydrogen embrittlement) and failure by cracking or blistering of the steel. The removal of the carbon from the steel results in decreased strength. A graph which shows the accepted limits for the use of carbon and low-alloy steels is used to determine the suitable materials for the equipment design [4]

- The ATR reactor
  - Autothermal reactor design is almost exclusively described in patent literature. In appendix 49 rough estimations are used to get an idea of the dimensions of the reactor. Fore more detailed design the reader is referred to patent literature
  - The design of the flame is crucial, but no information is found for the design. Information should be available in patents, but no examples are found.

- The gas/liquid separators
  - The gas/liquid separators are horizontal or vertical drums. Rules of thumb are obtained from literature to design the drums [5].

- The FT reactor
  - The FT reactor is designed according to a model obtained from literature. This model consists of three ‘phases’ for which mass

balances are made, these are: large bubbles, small bubbles and the liquid phase. The conversion is modeled with known kinetics and the throughput from design space 4.

- The distillation columns and stripping columns
  - The principal factor that determines the column diameter is the vapor flow-rate. The vapor velocity must be below that which would cause excessive liquid entrainment or a high pressure drop. An equation based on the Souders and Brown equation is used to estimate the maximum allowable superficial vapor velocities and hence the column areas and diameters
  - Information is gathered about different types of contacting plates that can be used for the columns. The most important types of plates that are taken into account are; sieve plates, bubble-cap plates and valve plates.

- The hydrocracker
  - Also the design of hydrocrackers is mostly described in patent literature. In appendix 57 a typical hydrocracker from industry is described to mention the most important features of the design of the hydrocracker. For further details reference is made to a number of patents. The hydrocracker sizing is mostly based upon the heat duties that are calculated in design space 4. During design space 4 it was decided to make the heat production in each catalyst bed equal. According to these calculations and a typical liquid hourly spaced velocity of industrial hydrocrackers the catalyst beds are sized.

- The isomerization reactor
  - There is not much information found about isomerization reactors in industry. This likely due to the fact that these reactors are not much used for similar applications. Most isomerization reactors used in industry are used to improve the octane number of gasoline. These reactors isomerize hydrocarbons with much smaller molecular weights. The isomerization reactor of the process is designed similar to the hydrocracker, because the only major differences between the hydrocracker and the isomerization reactor are the operating conditions and the type of catalyst that is used. These are described in chapter 6.

- The pumps, compressors and heat exchangers
  - The focus of the design of these pieces of equipment is to get an idea of what reasonable costs are for this kind of equipment
  - Information is gathered about the type of compressors and pumps that can be used in the process

- o Duties are obtained from the AspenPlus simuation
- o The most important features about the heat exchangers (transfer area and overall heat transfer coefficient) are obtained from a short-cut design method in AspenPlus. Information is also obtained about types of heat exchangers that are used in industry.

1.45.1 *Design tools to manipulate objects*

As in the previous design spaces there are design tools, which influence the choices that were made. In this design space these tools influence the choice of a certain type of equipment and the material that will be used. Also in this design space the criteria from the PIQUAR tool are used [R010] as criteria in decision-making e.g. in choosing the type of equipment and to evaluate the design.

The aim is to reach the production capacity, as efficiently and effectively as possible also here the same trade offs should be made between:

- Economics
- Product quality and quantity
- Safety
- Controllability and operability of the process
- Sustainability (type of material used)

With the help of these PIQUAR factors, taking into account the optimal choice of the type of unit and the material, the design is done.

With the help of the results from the Aspen tools, the throughputs and the heat duties and some other specifications for the units are then known for further sizing of the equipment.

Another tool that is important in this design space is the use of rules of thumb. In the scope of design is explained that it is not possible to design the equipment in great detail because of the available time and the large number of equipment. Therefore rules of thumb have been gathered during the phase where knowledge is gathered of this design space [5].

1.46 Synthesis

In this design space the synthesis part is focused on choosing a certain type of unit, which is most fit to handle the process conditions, while taking into account the important piquar factors. With the choice of the unit and with this its specifications, the size of the unit and the material of which the unit will be made is then determined. The synthesis of the equipment is described in the previous mentioned appendices. The main results are summarized in appendix 62, which gives the equipment data sheets.

Finally from the reports of the equipment sizing the economics of the design are then calculated. The units that are 'sized' and the units that were not sized, but are present in the design are included in the calculation by scaling techniques of the costs.

1.47 Analyses and evaluation

The pieces of equipment that are present in the process flow sheet are:

- Four pumps
- Four compressors,
- Sixteen heat exchangers,
- Three distillation columns, two of them containing strippers,
- Four reactors,
- Four vapor/liquid separators.

From the equipment sizing we can see that the largest units are the FT reactors and the fractionator. As said before the compressors are sized by calculating the work and steam requirements. These units are not all the units that should be present in the process if it would be developed. The pumps for instance are much less then in reality would be required, all cooling water streams would need a pump, and between most of the pipeline a pump should be installed. In the economic calculations in some cases it is tried to include these equipments, which were not visible in the flowsheet but in reality should be there, by multiplying the cost by a certain factor. This described in more detail in appendix 60: economic evaluation [R608].

The economics of the process can now be evaluated in this design space. The costs for process control are not taken into account yet, but it is assumed that these costs do not have a large impact on the analyses. A summary of the equipment costs is given in Table 6.

Table 6: Summary equipment costs

Description of equipment	Reference code	Costs [1998 10^3\$]
ATR	R1	61
Fischer-Tropsch reactor	R2	1,624
Isomerization reactor	R3	288
Hydrocracker	R4	486
Membrane separator 1	S1	487
Membrane separator 2	S2	43
Vapor/liquid separator 1	V1	48
Vapor/liquid separator 2	V2	17
Vapor/liquid separator 3	V4	10
Vapor/liquid separator 4	V7	14
Wax/md distillation column	C1	28
Preflash column	C2	112
Fractionator column	C3	254
Compressor 1	K3	845
Compressor 2	K1	1,775
Compressor 3	K2	1,586
Compressor 4	K5	56
Heat exchanger 1		326
Heat exchanger 2		987
Heat exchanger 3		560
Heat exchanger 4		292
Heat exchanger 5		107
Other heat exchangers		4,543
Pump 1	P1	12
Pump 2	P2	8
Pump 3	P3	15
Pump 4	P4	12
Other pumps	NA	188
	Total	**14,787**

A summary of the costs of utilities per year is given in Table 7.

Table 7: Cost of utilities per year

Type	Price ($/unit)	Amount (x)	Cost (10^3\$)
Steam* (ton)	17.2	-1,349,077	-23,204
Electricity (kwh)	0.18	1,098,578	198
Cooling water (m3)	0.08	2,354	0.2
		Total	**-23,006**

* Medium pressure steam

The raw material costs are given in Table 8.

Table 8: Raw material costs

Name	**Costs ($10^3$$)**
Natural gas	72,800
Oxygen (ton)	25,006
Catalysts	12,767
Total	**110,573**

The annual income from the products is presented in Table 9.

Table 9: annual income from products

Name	**Income ($10^3$$)**
Naphtha	15,199
Diesel	23,534
Kerosene	25,371
Total	64,104

From Table 6, Table 7, Table 8 and Table 9 the net cash flow can be calculated. The results are explained in more detail in appendix 64: economic evaluation. The main results are summarized in Table 10.

Table 10: Annual cash flow calculation

Type	**Amount ($10^3$$)**
Gross income	64,104
Operating costs	90,329
NCF	**-25,225**

As calculated the economics of the process are bad with the negative cash flow the process is unlikely to be feasible if the location is not special. In the future if the product prices changes or the any of the factors of the annual production costs changes in a positive manner the process could become feasible. Compared to last economic evaluation in design space 4 (chapter 6) the economics have improved due to the large amount of steam that is produced. If this steam can be sold or if electricity is produced from it are the economics of the process greatly improved.

1.47.1 Piquar evaluation

The overall piquar evaluation in this design space decreased compared to previous design space. The main factors that got a high average grade are product quality, team spirit and innovative design. For the product quality and quantity the requirements of the client are met, the combined syngas CO2 recycle is thought to be an innovative improvement in the design. Though because of bad judgment of time spend on DS4 which lead to shortage, the team still enthusiastically continued the design. The criteria return on investment, keeping deadlines and planning scored low because still there is a negative rate on return especially now with equipment costs included and because of the poor judgment of the time spent on DS4 a shortage of time originated. The economics however improved due to the large amount of steam that is produced. The results of the individual and team piquar can be found in appendix 6.

1.47.2 Safety

The safety of the process could again be done in this design space by making use of the DOW F&EI. Compared to the previous design the explosion index did not change much. The only data that was now available that first was not is the material of design of the units. The results are available in appendix 61: DOW fire & explosion index of DS 6.

1.48 Results

The results of the sizing of the equipment can be found in the following reports:

- Equipment design FT reactor [R601]
- Equipment design ATR reactor [R602]
- Equipment design Vapor/liquid separator [R603]
- Equipment design distillation columns [R604]
- Equipment design compressors and pumps [R605]
- Equipment design hydrocracker [R606]
- Equipment design isomerization reactor [R607]
- Process economic evaluation [R608]

A summary of the different equipments and their specifications can be found in the equipment specification and data sheet [App601].

1.49 Conclusions

The equipment design is done to have a have global idea of the geometry and specifications of the equipment that will be used. With the help of the design the equipment costs of the process can be calculated. A very important piece of equipment that is not designed is the membrane reactor.

But these costs should be taken into account more accurately, because membranes are very expensive units. From the design can be concluded that for the equipment costs, the fractionator and the FT reactors have the largest contributions. The heat requirements and the purchased costs of the compressors give an indication that they are also a mayor part of the costs of this process. The biggest costs of this process are the raw material costs. So for future development of this process the production costs (raw materials) should decrease. Although not all the equipment is designed to the desired degree of detail the team decided to propagate to the final design space, which is about integration of safety and controllability, because else no time is left for this design space. With the breakeven analyses we came to the conclusion that, because of the relative high increases that need to occur in the product and or raw material prices, there has to be a very large change in the current oil market for this process to earn back its investment at the end of its lifetime.

1.50 Literature

1. J. Grievink et.al., 2001, A framework for conceptual design of process plants.
2. R.K. Sinnott, Coulson & Richardson's chemical engineering volume 6, third edition, Butterworth & Heinemann, Oxford, 1999
3. J.M. Douglas, Conceptual design of chemical processes, McGraww-Hill, Boston, 1988
4. RH Perry, DW Green, Perry's chemical engineering handbook, 6^{th} edition, McGraw-Hill, New York, 1994
5. CR Branan, rules of thumb for chemical engineers, Gulf publishing company, Houston, 1994

Design space 7: systems integration

Summary

In this design space the safety systems and the control systems are integrated over the entire process. Safety and controllability have been an important issue for decisions in every preceding design space. In this design space the safety and controllability aspects of the process are further analyzed and a global picture of safety and controllability is obtained. A new hazard evaluation technique, HAZOP, is used for the first time in this design space. The controllability involves all the tasks that are necessary to safely control the process. The HAZOP analysis is closely related to the controllability. A number of appendices are generated that support the contents of this chapter:

- Appendix 63: HAZOP study [R701]
- Appendix 64: Applied control strategies [R702]
- Appendix 65: final flowsheet [P501]

The most important output of this design space is the final flowsheet with all the control schemes and the HAZOP study where a number of suggestions are done to improve the safety and controllability of the process.

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1.51 Scope of design space 7

This design space primarily aims at the integration of the safety systems and of control systems over the entire process. Integration of safety in this design space comprises hazard evaluation and design of safeguards to avoid identified hazards or to mitigate their effect. Safety has been an issue at every design space in the decision making for certain unit operations or types of equipment. At every design space a DOW fire & explosion index is made. Even so, it is very likely that some hazards still remain. These must be detected in this design space.

The types of objects that are taken under consideration in this design space are related to the control systems. The control systems are designed on a plant wide scale, plant wide control involves:

- Consistent placement of plant measurements and actuators
- Design of control loops for flows and conditions in individual equipment
- Control of product quality (plant wide co-ordinated)
- Optimizing production efficiency and profit
- Start-up and shut down procedures

1.51.1 *Battery limits, exchange streams, constraints:*

The battery limits of the objects in this design space are the use of only basic control systems. The goal of the design team is to show that the process is controllable and to indicate the start-up and shut down procedure. Advanced control schemes or control equipment are outside our battery limit. All the targets and constraints from the previous design spaces [DS0, DS 1, DS 2, DS3, DS4, DS5 and DS6] still apply for DS7. Additional targets and constraints are:

- The process flowsheet resulting form DS6 should not be changed anymore in this design space
- Controlled variables are designated
- Manipulated variables are designated
- Disturbances are designated and controlled
- Control performance targets are set
- Safety targets are set

1.51.2 *Design decision variables*

The design decision variables are related to how the plant is controlled. These design decision variables include:

- Function of equipment and elements
- Ports (mass, energy or information)
- Connectivity of control- and safety elements
- Type of equipment, and control- and safety elements.

The design decision variables result in the implementation of a control scheme in the flowsheet from design space 6. In this control scheme is made clear which manipulated variable control a certain controlled variable. In the scheme should also be made clear which safety precautions are taken to minimize a certain hazard. Additional information will be provided about the basic control and safety equipment that is used.

1.52 Knowledge of objects

The objects that are identified for this design space are:

- Equipment (e.g. relief valves)
- Elements for control and safety (sensors, actuators and controllers)
- Information streams
- Process- and utility streams set in previous design spaces
- Network of equipment, streams and control- & safety systems

The knowledge about the process- and utility streams is obtained from design space 4,5 and 6. The knowledge about the main hazard identifying tool HAZOP that is used in this design space is taken from literature and described in a separate document about hazard detection and control:

- Hazard detection and control [R701]

The knowledge that is necessary to design the control scheme is available in many literature sources. The most important information from these literature sources are suggested control schemes to accomplish the targets set in this design space. In a separate document about process control these different control schemes will be evaluated and a decision is made for the most favorable control scheme. These decisions are described in a separate report:

- Applied control strategies [R702]

1.52.1 *Design tools to manipulate objects*

For the identification of the hazards two tools are used:

- DOW fire & explosion index; the index is made for every design space and an assessment of the fire and explosion risk can be made with this index.
- HAZOP; HAZOP stands for Hazard and Operability study.

The HAZOP study is closely related to the controllability of the plant. A poorly operable process is usually also unsafe.

1.53 Synthesis

For the most recent DOW fire & explosion index reference is made to design space 6 [DS6].

The sequence of the synthesis of the process scheme is as follows:

- The team proposes a control scheme for the process
- HAZOP study is done to identify the remaining bad controllable process parameters that induce hazard
- The final control scheme is made according to the HAZOP study

The reasoning behind the control scheme selection is presented in Appendix 64: applied control strategies. The most important types of control that are used are feedback control and ratio control. As explained in the scope of design only basic control schemes are used to design the controllers. The HAZOP study is synthesized in a group brainstorm session with the help of guidewords to generate ideas. All the ideas are available in appendix 63: HAZOP study.

1.54 Analyses and evaluation

The complete flow scheme, which is the main output of this design space, shows that the process is controllable. A large number of the improvements that were generated during the HAZOP study are included as recommendations to improve the safety and controllability of the process. The hardware elements that are necessary for the controllability are not taken into account for the economic evaluation, because this evaluation is carried out in design space 6. Also no information about the prices for this kind of equipment is readily available to the team.

1.54.1 Piquar evaluation

The PIQUAR evaluation of design space 7 is the latest created PIQUAR evaluation of this report and shows the general feeling of the team about the quality of the design. The individual and team marks are available in appendix 6: PIQUAR. The results of the PIQUAR tool are described in more detail in the next chapter where the creativity and work processing tools are described. The quality of the design is improved compared to design space 6, because design space 7 showed that the process is controllable and operable. Besides the controllability also the safety improved because of the HAZOP study that was carried out. Also from this PIQUAR analysis is clear that the time planning and keeping deadlines was not good. The extra time that was taken for design space 4 could not be spend anymore for design space 7.

1.55 Results

The results of this design space are shown in the three appendices mentioned in the summary. These appendices show the control scheme as it is applied in the flowsheet, the reasoning behind the chosen flowsheet and the HAZOP study.

1.56 Conclusions

The results from design space 7 are taken as the final result of the design process. Design space 8 is omitted from the design process as agreed with the client and principal. The reasons for this are the time limit of the project and the fact that the topic of design space 8 (flowsheet optimization) is not a part of the present chemical engineering curriculum.

1.57 Literature

1. H.J. Pasman, S.M. Lemkowitz, Chemical risk management, Faculty of applied sciences, Delft university of technology, 2002

Creativity, Work Process &Tools Evaluation

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1.58 Introduction

At the kick-off meeting for this project, a number of methods that could enhance creativity were described; brainstorming, mind mapping, synectic thinking, TRIZ, incubation, visualization, constructive criticism, creating pleasant working atmosphere, watching deadlines and review meetings.

The group had the opportunity to put in practice many of these methods. Some of them proved to be effective, leading to a good creative atmosphere and enhancing our capacity for finding creative solutions in several situations during the design. Here, we will discuss the proposed methods and give examples of their application.

1.59 Methods and Techniques

1.59.1 Brainstorming

Brainstorming is the generation of ideas by a group. The starting point of our design was an initial design from a former group. At the start of each design space the team reviewed the findings and solutions from the former group.

After each team member had read the documents we kept a team meeting where we brainstormed for other solutions. We tried to think of as many alternatives for their design as possible. Sometimes this was useful and other times it wasn't. For example during the review of design space 1 from the former group (20-05-2003), we tried to think of new ideas. This turned out to be useless, because there were not many parameters left anymore.

From design 4 and later, brainstorm was widely used in the generation of new ideas and alternatives for the process. In DS 4, for example, brainstorm sections were performed in order to imagine different flow sheet configurations and connectivity between the streams. The combination of the tasks in DS4 was also made after brainstorm sections.

In DS5 we have also made use of brainstorm in order to come with different configurations for the heat exchanger network. The same happened in DS7, where a brainstorm session was held in order make a list of possible problems that could occur during the operation of the plant.

1.59.2 Mind mapping

Mind mapping means that the idea generation is done in a specific way and that the ideas are noted in a specific way. We didn't use mind mapping explicitly.

1.59.3 Synectic thinking

At the brainstorm session we tried to use synectic thinking. By this method we try to link the different thoughts of each group member and maybe we can generate some new ideas form that. It is also possible to try the link the problem to a different problem that is based on the same principle.

During this project, we have always paid attention in the ideas of each group member. In some cases, we have used the principles of the idea from one group member in order to develop a new concept or idea.

1.59.4 TRIZ

TRIZ is a combination of algorithms and principles. A key concept is for example how to handle contradictions. Traditionally, trade-off or compromise is used to handle contradictions. TRIZ always seeks a solution without compromise. In this way the situation where a compromise has to be made (which could even be worse than picking one of the articles) could be avoided. This can lead to a final solution, which is even better than the compromise (the best features of the ideas are combined in one solution).

We recognized TRIZ in our idea generation during the selection of the best technology for synthesis gas production. The two main conventional technologies for synthesis gas production are steam reforming and autothermal reforming. We investigated the available technologies that can combine the advantages of both technologies. Therefore we initially decided to investigate combined reforming (steam reforming after an ATR) and GHR (a steam reforming reactor that is heated with the exit gasses of an ATR reactor). Our analysis made us decide that GHR was not a good option after all (the required product ratio could not be achieved) and combined reforming could be used. Therefore we worked out the combined reforming idea. However at stage 7 of the delft design matrix cycle (go or no-go), we decided that we would not continue with the combined reforming to the next level. This was mainly due to the fact that we would produce too much hydrogen that we couldn't use and that there were still quite some uncertainties about this technology.

This method was widely used in almost all design spaces, especially in DS4, where we integrated the strong points of different possible flowsheets. This way, we tried to eliminate the weak points of the proposed flowsheets, while enhancing their positive points.

1.59.5 <u>Incubation</u>

Incubation turned out to be very effective if we didn't make progress. This was no surprise for the team members, because we all recognize that work should be varied with more relaxing activities. Sometimes a 'fresh' memory is necessary to go on. During this project, we have experienced many situations were we could not go further with a problem because of lack on information. This happened, for example, while dimensioning the Fischer-Tropsch reactor and distillation columns. In these cases, the group usually decided to take a pause, talk and (try to) relax. Then, we carried out some discussion with all team members in order to try to find a solution for the problem. If we could not achieve any improvement after this discussion, we usually left the problem behind for some hours or for the following day.

1.59.6 <u>Visualization</u>

Visualization is used many times during team meetings. Some examples of the application of this method are given below:

DS2: Alternatives are far clearer if a quick blockscheme is drawn to support the story. During design space 2 each team member was assigned a section where he should have more expertise than the other team members. During the team meetings, where each team member explained the basics about his technology, blockschemes were almost always used to clarify and to clarify the complete blockscheme.

DS4: Visualization was used to compare different alternative flowsheets. The alternative flowsheets were printed and put on the table or hanged on the wall and we could draw our new ideas on the printed flowsheets. A blackboard was also used to draw different configurations for the product upgrade section.

DS5: Visualization was a very important tool in order to develop the heat exchanger network.

DS7: Visualization was essential in the design of the control system.

1.59.7 Constructive criticism

At the preparation of the kick-off meeting the team discussed the importance of constructive criticism. We all felt that it was very important to support every idea, even if it is really strange. However no exceptional strange ideas emerged during team meetings, we all have the feeling that every idea is treated seriously and everyone is allowed to give his opinion freely without immediately being criticized.

During the process design, we experienced some situations were one or two group members did not agree with the idea of the rest of the group. In all situations, we were able to solve the difference of opinion with constructive criticism and we could always come to a consensus without problems.

1.59.8 Pleasant working atmosphere

The working sphere is good. Because we work with a small team, the team communication lines are very short. For important decisions and task distributions formal meetings are organized. But also discussion takes place during coffee time etc. We try to maintain this, to our opinion, good balance between these two.

1.59.9 *Keeping deadlines*

In the beginning of the project we have made a planning, reserving a certain time for each design space. Then, on the beginning of each design space, we made a new planning with deadlines for the delivery of the reports.

It was quite difficult for the group to follow the planed deadlines. The main cause of this problem is that the group spent too much time on design space 4, leaving not too much time for other important tasks.

In fact, this caused some problems in the whole planning, because we have start with DS5 and DS 6 while DS4 was not finished.

1.59.10 *Review meetings*

During the kick-off meeting, our creativity coach suggested that a good way to promote the working process is to keep small informal review meetings at the end of each day. The team tried this and noticed that it is a good and very useful excuse to keep a break at the end of each day. In this way we can keep better track on how the work is going. Review meetings were held during the whole project and it proved to be very important in order to keep every group member informed about the advances and the problems occurring in all parts of the project.

1.59.11 *The Delft Design Matrix*

The general design method that is used is the Delft Design Matrix (DDM) [Grievink, 2001]. The DDM is a design method that gives guidance to the design teams throughout the whole design process. The DDM is divided into 8 different design spaces that on its turn consist of 7 generic cycles (scope of design, knowledge of objects, synthesis, analysis, evaluation, report and finally go or no-go). The separation of the design process in these subspaces gives more room for implementing creativity and induces a more efficient approach.

The approach used by the design matrix is very objective and helpful in the sense of promoting creativity and innovation in the process design. The definition of tasks and changes of state in DS4 and the later integration of these tasks in unit operations give a lot of space for innovation. It is much better to list and analyze the tasks apart and leave the integration of them for a later stage. This keeps the mind more open for different possibilities. In the product upgrading section, for example, hydrocracking and isomarization could be performed in one single reactor, but this would lead to the cracking of valuable valuable product to lighter hydrocarbons. It was than decided to perform these two tasks in two separate reactors and crack only heavy products. Another example of innovation that was in a certain sense promoted by the use of DDM is the design of connection of the recycle streams.

The DDM makes it possible to make a detailed planning for each design space. The structures of the design spaces are very helpful in determining what will and what will not be done in each design space. It also gives an good overview of the tools and variables that can be used in each phase of the design.

The group had some problem with the planning of the project. Some design spaces may take much more time than the others and the group did not make a good estimation of the time necessary for design space 4. For this reason, some design spaces had to be carried out simultaneously.

Sometimes it was not easy to separate tasks from different design spaces. This was the case, for example, for DS4 and DS6 and for DS5 and DS6. Constraints in the equipment design may influence the flow pattern, the contacting area etc. For the Fischer-Tropsch reactor, it is difficult to determine contacting area and reaction rate independently of the reactor or the catalyst type.

In the beginning of the project the group could has delivered the BOD with a small delay. It was caused by the fact that the format of the BOD report is completely different from the format of the DS reports. After making several reports for the first design spaces, the group still had a lot of work to do in order to finish the BOD. It would be better to change the first DS or adapt the BOD in such a way that they would be compatible with each other.

1.59.12 AAA

Advanced Activity Assistant (AAA) consists of a planning tool that helps the group to keep track of the tasks as well as of the outputs of the tasks and their deadlines. The main futures of the AAA are:

- Activity description
- Goal of activity
- Responsible person / group
- Start date
- Deadline
- Input and output information

Since the beginning of the project, the group tried to make plannings using the AAA tool. It was also a good for the communication and division of tasks. It took us some precious time to update the AAA file, sometimes it had to be done with some delay, but we succeeded in keeping it updated eventually. The AAA excel file can be found in Appendix 3 AAA.xls

1.59.13 PIQUAR

When designing a process using the DDM it is important to make sure the quality is checked during every stage. A tool that can be used to describe the quality of the design according to the designers is the PIQUAR (Plant design Improvement by QUAlity Review) tool. This tool uses a number of criteria that are to be set by the designing team and the principal. Every criterion should be awarded a weighing factor depending on its importance in the design. For each Design Space the designers should give a grade from 0 to 1, zero meaning this part of the design is absolutely not to his or her satisfaction and one meaning this part is perfectly covered in the design. Using the weighing factors a PIQUAR number can be calculated for the design. This quantifies the designer's feeling about the project.

1.59.13.1 Criteria

The PIQUAR criteria are arranged in descending order of priority.

Product quality and quantity
This point refers to the quality and quantity of the product and the by-products. Are the specifications set by the principal regarding quantity and quality met? Is there room for improving the quality of the products?

Safety
The safety criterion includes the safety for the surroundings, employers and the intrinsic safety.

Sustainability
This relates to the feeling about the sustainability of the design. In this factor the following points should be taken into account: durability, effect on environment and the product life cycle. Are the environmental legislations set by the local authorities met?

Low production cost of end-product

One of the most important economic factors is the cost of your end-product. Do you feel the cost is too high? Is the cost competitive? Are there still opportunities to reduce the cost of the end product?

Operability
This criterion deals with the controllability, flexibility, stability, optimality, switchability and availability of the process. Is there a chance a runaway could occur? Are a large number of controllers necessary to keep the process stable? Does the breakdown of controller systems have serious consequences? Are the resources, the knowledge and manpower available? Is it possible to switch between products if the market demands this? Are startup and shutdown safe?

Good communication and documentation
During the project communication between group members is important. Is it clear what every team member is doing? Do you have the feeling the meetings are useful? Furthermore the documentation of the work done should be easily accessible and clear. Is it clear to you where to find work that has been done? Are you satisfied with the quality of the reports? Are the decisions explicit and can they be repeated?

Return on Investment
The return on investment is the most important factor for investors. This should be as high as possible. Do you think the return on investment is high enough? Is it attractive enough for investments? Are there still opportunities to raise this number?

Maximum availability
This factor discuses the availability of the plant for production. Is the downtime for the plant kept to a minimum? Are there any units that are very vulnerable and could cause downtime for the entire plant?

Innovative design
In the designing of this process a number of creativity tools are used. The goal of these tools is to create an innovative design. Do you feel the design is innovative? Are the results of the creative tools helping you make an innovative design?

Keeping deadlines and good planning
To stay on schedule deadlines that are agreed upon should be kept and good planning is necessary.

Use of tools (DDM, AAA, PIQUAR and creativity tools)
While designing the process a number of tools are used. Do you feel these tools are useful? Are they used correctly and frequently enough?

Team spirit during design
For this point, take in to account your general feeling about the teamwork. Is every team member functioning as agreed? Are you happy with your position in the team? Does the team create a good working environment for you?

1.59.13.2 PIQUAR Factors

The former group and the principle already specified the criteria and the weighing factors that we will use during this project.
The principal already indicated the order of importance. The factors used for the PIQUAR evaluation are listed in Table 11.

Table 11. PIQUAR weighing factors.

PIQUAR Factor	Weighing Factor
Product quality and quantity	0.202
Safety	0.154
Sustainability	0.115
Low production cost of end-product	0.106
Operability	0.096
Good communication and documentation	0.077
Return on Investment	0.067
Maximum availability	0.048
Innovative design	0.048
Keeping deadlines and good planning	0.039
Use of tools (DDM, AAA, creativity tools)	0.026
Team spirit during design	0.022

1.59.13.3 Application

Since the early stages of the process design we have made use of the PIQUAR tool in order to help us making some decisions and evaluating the quality of the project. The selection of the syngas production unit was made based on a PIQUAR analysis of the different reactor options. The same happened for important decisions as the choice of the FT reactor, the flowsheet selection, the hydrogen purification unit etc. These PIQUAR analyses can be found in the appendices over equipment and flowsheet selection.

At the end of each design space we have performed a PIQUAR evaluation of the project, which can be found in Appendix 6. The result for this evaluation is presented in the figure below:

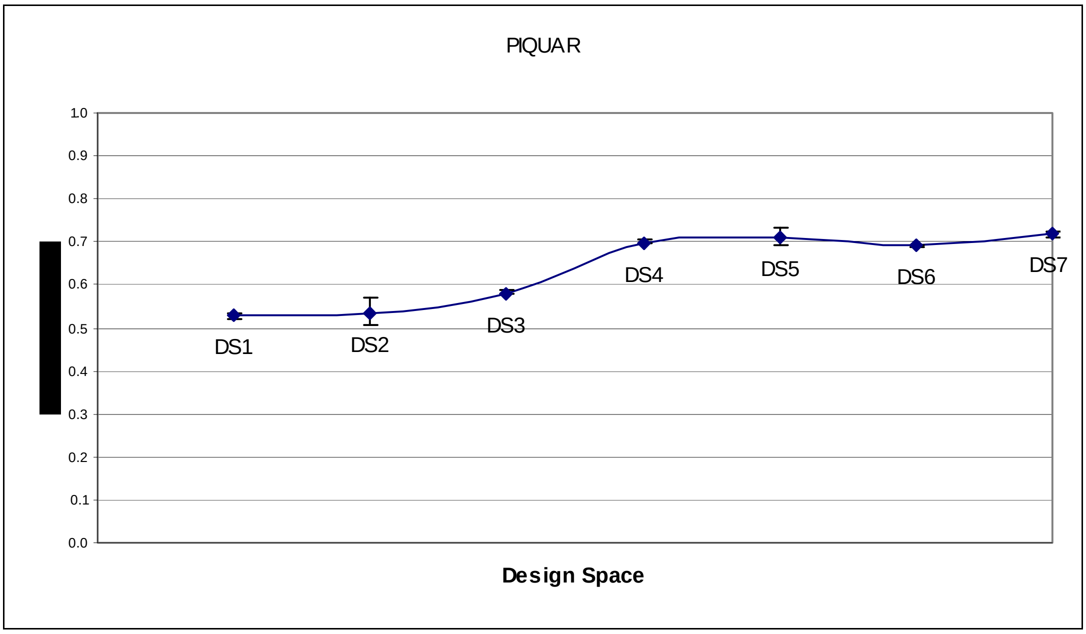

Figure 8: PIQUAR evaluation for Design Spaces

This plot shows a clear increase in the design quality in the course of the project. The line shows a sharper increase in the design quality from DS3 to DS4. After that, it remains almost constant from DS4 to DS7. The most important improvement in DS7 was the operability of the plant. In DS5 we achieved improvement in production cost reduction by integrating heat streams and exporting medium pressure steam.

Although it is not easy to quantify some aspects of the process, the PIQUAR tool is valuable in the sense that it provides us a general idea of the design quality. Large decreases in the project quality after a design space should require a deeper study of the PIQUAR factors in order to discover where the problem is and how it could be solved.

1.60 Conclusion and Recommendations

The design of creative and innovative process may be enhanced when the team makes use of techniques as those commented in this report. For this project, they have proved to be a valuable tool in de design process. Tools like AAA and PIQUAR should also become a standard in CPD projects. The first improves the project planning and communication, whole last one helps the designers to judge the quality and the development of the project.

We believe that the Delft Design Matrix is a very effective tool that can be used to promote creativity and innovation in process design. It is very helpful as a guidance tool for the CPD project and the small problems experienced by the group could be solved for later versions. After this first experience with the Delft Design Matrix, it will be easier to apply this method later on, as we already have a very good idea of the structure of each design space and the way it should be followed.

1.61 Literature

1. Herder, P.M. and Weijnen, M.P.C. (1999); Assessment of the quality of the design process and the design of chemical plants with PIQUAR, Computers & Industrial Engineering, Vol. 37, No. 1-2, October, 1999

Conclusions and recommendations

During the design of the process a number of strengths and weaknesses are encountered. In this chapter these points are summarized. Furthermore suggestions are given to improve specific weak points.

The strengths of the design are mainly:

- The autothermal reactor generates a large amount of heat that can be used to heat various large process streams as described in chapter 7 (design space 5).
- Product destruction by cracking is minimized by implementing an isomerization reactor. If the hydrocracking could be performed selective for only heavy products and the throughput is small enough for one reactor, a single reactor would possibly be more efficient. However the throughput of the process makes two reactors sensible and no detailed information about a catalyst that could hydrocrack selective only heavy hydrocarbons was available to the team.

- The modelling of the FT reactor is based on a reasonable model and the design of the FT reactor is performed fairly detailed
- The major part of the steam that is produced by the FT reactor can be used to generate electricity or to sell it to the steam supplier. This enhances the economic potential of the process as described in chapter 8 (design space 6).
- The process seems good controllable with basic control schemes as described in design space 7.
- The recycle of the carbon dioxide and syntheses gas are combined and the separation is of these gasses is carried out in existing columns. This decreases the amount and complexity of separation steps.
- The purity of the products is more than enough
- The flexibility of the process makes it possible to tailor the process products to one of the three main products. Only wax is cracked and by changing the operating conditions of the hydrocracker the selectivity towards a desired product can be enhanced without opposing the risk of significantly cracking of products. Besides by changing the separation performance of column C1 more diesel can be send to the hydrocracker and cracked to lighter products if desired.
- The products are environmental friendly compared to competitive products; they contain virtually no sulphur of nitrogen.

The weaknesses of the design are mainly:

- The LPG that is produced in the Fischer-Tropsch reactor and the hydrocracking is for a large part burned in the ATR. This is not only unsustainable, but it also decreases the economic potential of the process (LPG can't be sold as a by-product). It should be noted that the LPG can be recovered, but due to the time limit of the project and the nature of the project description the required equipment and utilities are not designed.
- The separation of the carbon dioxide and synthesis gas is carried out at relative low pressure. The consequence is that larger compressor costs are required to bring the recycle gasses to the required pressure.
- A number of pieces of equipment are not designed to a satisfactory degree of detail in design space 6 (chapter 8) due to time limits and the availability of the information in literature. Equipment that is not designed very detailed is for example:
  - Heat exchangers
  - Pumps
  - Compressors
  - ATR
  - Membranes

- Some transfer rates could not be modelled very detailed, because no suitable kinetic model was found, these models are mainly related to the membranes and the hydrocracker/isomerization reactor. The latter two reactors are modelled according to a typical product distribution from equivalent equipment in industry. The disadvantage of this approach that no knowledge is obtained from the behaviour of the reactor if for example the operating conditions change in the reactor.

- The design of crude distillations turned out to be a very specialized and time-consuming activity. The modelling is carried out solely with the assistance of engineering software. The disadvantage of this approach is that no large physical comprehension of the technical phenomena is obtained. Therefore there is little comparison possible with other calculations.

- During start-up a large amount of additional heat sources are necessary, because the outlet stream of the ATR supplies a large part of the heat in the process. A furnace might be necessary only for start-up.

- Pressure drops in equipment is based on rough estimations. More detailed modelling for the pressure drop would give a better estimation for pressure drops.

The major risks (technical and financial) are identified during the various design spaces and are summarized in this chapter. The greatest risks of the process are:

- The economics of the process depends very much on the availability of petroleum feedstock. If for example oil becomes easily available on the market the process might become economical unfeasible very rapidly.

- The ATR is rated to have the highest fire & explosion risk. The presence of flammable and explosive components with oxygen at high the highest temperature and pressure in the process is the cause of this high risk. However the technology is proven many times in industrial practice and can be operated smoothly with the right precautions. A number of precautions are identified in the HAZOP study.

- The reactions that occur in the Fischer-Tropsch reactor are comparable to polymerization reactions. The large heat production can ignite a runaway in the reactor. Heat removal is essential in this reactor as well as safety measures to stop the reaction as quickly as possible. These safety measures are suggested in the HAZOP study.

- Using cobalt as catalyst induces some financial risks. The global cobalt prices fluctuate and are not very predictive

- There is no protection against catalyst poisoning components. If for example sulphur is present in the natural gas stream the process won't be able to operate sufficiently. Good knowledge about the composition of the natural gas feed stream is necessary.

- The large amounts of contaminated wastewater can have a significant effect on the local environment. These wastewater streams should be processed with care.

- A large waste stream of the process is carbon dioxide. The emissions of carbon dioxide are a hot environmental topic at the moment. No strict guidelines are available at the moment for the emission of carbon dioxide as described in chapter 3 (design space 1). However it is very good possible that more severe guidelines will emerge with the economical lifetime of the plant.

Based upon the weaknesses and technical and financial risks that are identified in this chapter a number of recommendations are made by the team, these are:

- Separating the LPG from the recycle gas stream. This will enhance the sustainability (less LPG burning) and improve the economical potential of the process (LPG can be sold as a high value by-product).

- More details about the kinetics of the hydrocracker and hydro-isomerization reactor are preferable, because these will increase the modelling accuracy of the reactors. Also lab scale experiments are necessary to validate the assumptions made in this conceptual design.

- The design of the two membranes should be carried out more accurate to validate the assumptions made during the design. Little knowledge is available about the membranes

- Simulate process dynamics to investigate the dynamic behaviour for process control.

- Investigate the possible economic benefits of separating the recycle gasses at high pressure. During design the team used sensitivity analysis to investigate the feasibility of separating the Fischer-Tropsch gasses at high pressure, but it turned out to be difficult to prevent naphtha from entering the gas stream (naphtha should not be burned in the ATR because naphtha is part of the product capacity). High-pressure distillation could be an option to save compression costs.

- The economic viability of the process can be enhanced if more high-value chemicals are produced.
- Determining the pressure drop in more detail would improve the quality of the model.
- Short-cut models are used to model the distillation columns. Using more rigorous models improve the flexibility of the model.
- The ATR should be designed in more detail or a patent should be used to construct the ATR. Especially the design of the flame is important.