CPD NR3259

Conceptual Process Design

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

Subject

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TU Delft

Faculteit der Scheikundige Technologie en der Materiaalkunde

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Hydroisomerization of n-Heptane using Zeolite Membrane Separation Technology

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SUMMARY

Almost all octane boosters, which were introduced to enhance the RON, will be banned in the future because of environmental reasons. Therefore, the aim of this project is to develop a conceptual process design for the hydroisomerization of n-heptane, in order to enhance the octane number. It is the goal to convert n-heptane into multibranched isomers, preferably dimethylpentanes and trimethylbutane, to produce a product with an octane number (RON) between 90-95. The n-heptane hydroisomerization unit will be operating as an alternative to the existing alkylation and catalytic reforming processes and the isomerized product will be added to the gasoline blending pool. The feed of the process is coming from the hydrotreater, which currently goes to the catalytic reformer. This process does not exist, however comparable processes like C5/C6 do exist.

In this conceptual process design the kinetics are estimated, by fitting the available experimental results. These kinetic results are used in the reactor design. Also all the required separation steps, the design of all necessary heat exchangers, pressure changers and heat integration by pinch technology are covered in this CPD. The storage of feed and products is not taken into account. A HAZOP and a FE&I study is performed for this process.

This conceptual process design shows, that by using the latest membrane separation technology, a heptane hydroisomerization plant can be built. All unit operations are technically realizable and have realistic dimensions. A ZMS-5 membrane with a total area of 20,000 m^2 is used for the separation of the product isomers. It is placed in the channels of a cross-flow monolith which has a volume of 50 m^3. A total amount of 317500 tonne/a feed is processed from which is 77000 tonne/a, product is formed. The octane number of the product is 92. This means a product yield of 4.1 tonne feed per tonne product. The plant is on stream for 350 days a year, so maintenance can be done for 15 days a year, the on-stream factor is therefore 0.96. The selectivity towards the desired product 2,2,3-TMB is 20%. The conversion of n-heptane in the first reactor is 49% and the conversion of 2,4-DMP in the second reactor is 41%. The safety study showed moderate degree of hazard.

The total investment is 88.6 Mfl, the operation costs are 197 Mfl/a while the net income is 4.6 Mfl/a. The plant has an economical lifetime of 10 years. The startup time is 2 years. The economic evaluation indicates a negative cumulative cash flow during the 10-year operational life of the plant, given the current prices for feed and products. A product price increase of 6.4 percent is needed to attain a positive cash flow. Another possibility is to reduce the feed price with 10.5 %. The operating costs per tonne product are 2,559 fl/tonne. The investment costs per tonne product produced in 10 years are 114.8 fl/tonne. The income is very sensitive to feed and product prices, in contrast to investment and operating costs.

One of the limitations of this conceptual process design is the relatively large uncertainty in the parameters that were used to simulate the reactors and membranes. Therefore it is recommended to investigate the catalysts at the specific compounds and varying temperatures, while the membranes need to be investigated for the relevant mixtures of components. The original feed from the hydrotreater is simplified, because the kinetic model is based on conversions of linear C7. It is especially recommended to investigate the behavior of cyclic and aromatic compounds in this process. Attention should be paid to a better estimation than the rough estimation of the product- and feed prices, which are based on current gasoline prices and RON numbers in this report.

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1. INTRODUCTION

In spite of all major innovations in the automotive industry over the past decades, today's cars still run on gasoline with a minimum octane number of 95. This requirement for gasoline is an inseparable consequence of the internal combustion engine, which still drives 100% of the current car fleet. And, it will keep on doing so in the coming years, before alternative engines enter the market.

The refiner's job is to deliver a gasoline product with high enough octane number, while the octane number of the products obtained by classical crude oil fractionating is way below this specification. In the past, lead-containing compounds were introduced to enhance the octane number (like tetraethyllead). These compounds have a severe impact on the environment and were banned. Other octane boosters were introduced, like MTBE (methyl-tertiary-butylether). Again, government policy has forced use of MTBE back because of its low biodegradability. In response to this oil refineries intensified their reforming processes, in which linear molecules (paraffins) are converted to cyclic compounds (aromatics), which have a high octane number. As a side product lots of hydrogen is produced which in turn is extremely valuable in the refinery process. The major drawback of aromatics is however their high toxicity to man and to our ecosystem. The way it looks now is that use of aromatics in gasoline will be confined dramatically by legislation before the end of this decade. ① → 90

It is the challenge for the oil industry to anticipate these upcoming regulations by developing new processes that generate high octane number gasoline, yet do not violate these new governmental product specifications. In view of this, refineries have implemented the hydroisomerization process that converts linear paraffins to branched molecules, resulting in a major increase in octane number. This is already state-of-the-art technology for C5/C6 fractions, however for C7 this is not the case. The big challenge in C7 isomerization is to overcome product cracking, which is much more pronounced than in C5/C6 isomerization. The reward is high: By converting n-heptane to 2,2,3-trimethylbutane the octane number increases over 100 points.

The main objective of this project is to develop a conceptual process design (CPD) for the hydroisomerization of n-heptane, in order to enhance the octane number. It is the goal to convert n-heptane into multibranched isomers, preferably dimethylpentanes and trimethylbutane, to produce a product with an octane number (RON) between 90-95. The n-heptane hydroisomerization unit will be operating as an alternative to the existing alkylation and catalytic reforming processes and the isomerized product will be added to the gasoline blending pool (see the refinery scheme in Appendix IV). Currently in the common practice, naphtha is processed in the hydrotreater and then the pentane/hexane rich (C5/C6) stream is processed in the C5/C6 isomerization unit and the heavier alkanes are send to the catalytic reformer. The feed for the n-heptane hydroisomerization unit in this conceptual process design will be the n-heptane-rich stream, which currently goes to the catalytic reformer.

This conceptual process design will cover the estimation of the kinetics. These kinetic results will be used in the reactor design. Also all the required separation steps, the design of all necessary heat exchangers, pressure changers and heat integration by pinch technology is covered in this CPD. The storage of feed and products is not taken into account. A HAZOP and a FE&I study is performed for this process. The process is evaluated for economic potential.

2. PROCESS OPTIONS & SELECTION

There are no existing processes or process designs for the hydroisomerization of n-heptane. Process design and operating plants for the hydroisomerization of pentane/hexane do exist. Because the reaction mechanism of the hydroisomerization of n-heptane is similar to that of C_5/C_6, the optional process for the hydroisomerization can be based on processes for the hydroisomerization of C_5/C_6.

The processing options for isomerization of C_5 and C_6 are differentiated by catalyst type, once-through hydrocarbon flow or a recycle flow of hydrocarbon and whether the separation for hydrocarbon recycle is carried out by fractionation or by molecular sieve adsorption techniques. An overview of the most important processes can be found in Table 2-1.
A more detailed process description is given in Appendix 21.

Table 2-1: Isomerization process options, catalysts and separation techniques.

Process	Catalyst	Flowscheme	Separation technique	Developed by	RON	Yield vol-%
Penex	Chlorided Alumina	Once-through		UOP	82-85	100
		Recycle	DIH	UOP	87-89	98-99
		Recycle	Molex	UOP	87-90	100
Isomerization process BP	Chlorided Alumina	Recycle	Molecular adsorption	BP	85	99
Hysomer	Zeolitic	Once-through		Shell	82	97-98
Zeolitic	Zeolitic	Once-through			78-80	97-98
TIP	Zeolitic	Recycle	IsoSiv	Shell / Union Carbide	87-89	97-98
Par-Isom	Novel Metal Oxide	Once-through	DIP/DIH IsoSiv/Molex			

Although none of these currently operational processes make use of membrane technology, some aspects of these processes can still be used in the conceptual process design.

2.1 PROCESS OPTIONS

Based on currently operating processes (Appendix 21) several process options can be evaluated for the conceptual process design of the hydroisomerization op heptane. These process options have been summarized in Table 2-2 and are judged on five aspects: investment costs, operational costs, product yield, product RON and ease of operation.

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Table 2-2: Process Options

Option	Investment	Operational Costs	Product Yield	Product RON	Continuity / Operability
1 Reactor	+	+	–	–	+
2 Reactors	–	+	++	+	+
Distillation	+	– –	–	–	+
Membrane	–	+	+	+	+
Absorption	–	–	+	+	–
Once Through	+	+	– –	–	+
Recycle	–	–	++	+	+

+ means better, – means worse

2.2 SELECTION

Because product RON is the most important selection criterion, the following options have been chosen: 2 Reactors with recycle and membrane separation technology.

Reactor
The reaction section of present hydroisomerization processes (C5/C6) generally consists of one reactor, where isomerization occurs. It is necessary to separate the reaction section into 2 reactors, because the sequential reactions (n-heptane → monobranched + dibranched isomer → tribranched isomer) require different acid strengths of the catalyst. If the catalyst is too acidic, cracking of dibranched alkanes is enhanced, which is undesired. If the catalyst is a too weak acid the isomerization reaction does not proceed appropriately (see reaction kinetics). In this conceptual process design the reaction section will contain two reactors:

1. The first reactor where the reaction of n-heptane to mono- and dibranched isomers occurs
2. The second reactor where the reaction of specific dibranched heptane isomer (2,4 DMP) to tribranched isomer (2,2,3 TMB) occurs

Table 2-3: Kinetic Diameter and Boiling Point of n-Heptane and its Isomers

Molecule		Boiling point (°C)	Kinetic diameter (Å)
n-heptane	n-C7	98.5	4.2
2-methylhexane	2-MHx	90.0	5.0
3-methylhexane	3-MHx	92.0	5.0
3-ethylpentane	3-EP	93.5	5.0
2,3-dimethylpentane	2,3-DMP	89.7	5.0
2,4-dimethylpentane	2,4-DMP	80.4	5.0
2,2-dimethylpentane	2,2-DMP	79.2	6.0
3,3-dimethylpentane	3,3-DMP	86.0	6.0
2,2,3-trimethylbutane	2,2,3-TMB	80.8	6.0

Separation

- Feed treatment
  The largest portion of the feedstock is C6, C7 and C8 alkanes. These fractions are n-alkanes, isoalkanes and cycloalkanes. To separate the C7 fraction from the lighter and heavier components use is made of two distillation columns, a tailing and a topping column. The preferable feedstock should not contain water and hydrogensulfide because these will poison the catalysts.

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To separate the C7 isomer mixture into a fraction, which is destined for the first reactor and one for the second reactor, a distillation column will be used. The objective is to send the 2,4-DMP to the second reactor and the methylhexanes back to the first reactor. As can be seen from Table 2-3, isomer separation by distillation is possible. However, separation based on kinetic diameter is no good option here.

- Product
  As the conversion to the desired products is never 100% because of the thermodynamic equilibrium a recycle stream is necessary to obtain reasonable yields. The objective is to selectively remove the product (2,2,3-TMB) from the isomer mixture. This can be accomplished by using a membrane that retains all molecules with a kinetic diameter larger than 5 Angstrom. Consequently, the 2,2-DMP and 3,3-DMP will also end up in the product stream, but this is not a big problem since these compounds also have high octane numbers..

- Hydrogen separation/recycle
  Hydrogen is needed as a co-catalyst and to suppress cracking reactions. The hydrogen that is consumed by cracking needs to be replaced by make-up hydrogen. Most of the processes operate under a high hydrogen partial pressure, of which most is still present at the reactor exit, therefore it will be recycled. Hydrogen separation membranes are currently state-of-the-art and will be implemented without many difficulties.

Catalysts

In principle, there are two types of catalysts for skeletal isomerization of paraffins via carbenium or carbonium ions as intermediates [15]: monofunctional acidic catalysts and bifunctional catalysts that combine the acidic function with the hydrogenation-dehydrogenation function of a metal.

For this process there are 2 catalysts chosen:

- In the first reaction unit, where n-heptane reacts to mono- and dibranched isomers, the strong-acidic zeolite-based Pt/Hbeta with 0.5 w% Pt will be used as a (bifunctional) catalyst. This catalyst was chosen, because it had the highest conversion and selectivity to isomerization, and thus the least cracking. (See Appendix 25)
- In the second reaction unit, where only certain dibranched isomers react to tribranched isomer (2,2,3 TMB), the medium/weak-acidic amorphous silica/alumina with 5 w% Ni will be used as catalyst. This catalyst is chosen because it was the only catalyst where some experimental data was available, and it was specifically tested for the conversion of dibranched to tribranched molecules. (See Appendix 25)

3. BASIS OF DESIGN

In this chapter, the complete Basis of Design of the process is given.

3.1 DESCRIPTION OF THE DESIGN

The main objective of this project is to develop a conceptual process design for the hydroisomerization of n-heptane, in order to enhance the octane number. It is the goal to convert n-heptane into multibranched isomers, preferably dimethylpentanes and trimethylbutane, to produce a product with an octane number (RON) between 90-95. The conceptual process design will be based on studies on a molecular scale.

As a consequence of environmental concerns, the lead, MTBE and benzene level in gasoline has to be drastically reduced (or sometimes even banned) while keeping or even increasing the octane ratings. In petroleum refining the isomerization of light paraffins has been practiced for years [8], with the purpose of upgrading low octane number Straight Run Naphtha (SRN), in order to meet the increasing demand for high-octane unleaded gasoline and the environmental protection regulations for phasing out lead additives. SRN consists mainly of normal and monobranched paraffins. A large number of scientific papers have been published on the isomerization of light paraffins (e.g. n-pentane/n-hexane). Little has been reported on heavier ones (n-heptane and higher), although they also represent a potential feedstock for octane number enhancement. A reason for the lack of reports on hydroisomerization of n-parrafins higher than n-heptane is probably because of the cracking that occurs during isomerization of paraffins with 7 or more carbon atoms. Currently there do exist process designs and operating hydroisomerization plants [16] for light paraffins (e.g. TIP process, Hysomer process). There are several studies about n-heptane hydroisomerization, but there is no existing conceptual process design for a n-heptane hydroisomerization process.

Nowadays, a process design for n-heptane is possible, because of new technologies such as membrane separation technology. Also environmental reasons are driving forces behind developments in hydroisomerization of n-paraffins. Previously n-heptane was sent to the catalytic reformer to produce aromatics, which are major contributors to the gasoline blending pool.

The n-heptane hydroisomerization unit will be operating as an alternative to the existing alkylation and catalytic reforming processes and the isomerized product will be added to the gasoline blending pool (see the refinery scheme in Appendix 22). Currently, it is common practice, that is naphtha processed in the hydrotreater and then the pentane/hexane rich (C5/C6) stream is processed in the C5/C6 isomerization unit and the heavier alkanes are send to the catalytic reformer. The feed for the n-heptane hydroisomerization unit in this conceptual process design will be the n-heptane-rich stream, which currently goes to the catalytic reformer (See refinery scheme in Appendix 22). This conceptual process design will cover the estimation of the kinetics, by fitting the available experimental results. These kinetic results will be used in the reactor design. Also all the required separation steps, the design of all necessary heat exchangers, pressure changers and heat integration by pinch technology and a safety study is covered in this CPD. The storage of feed and products is not taken into account.

3.2 PROCESS DEFINITION

3.2.1 Process Options

There are no existing processes or process designs for the hydroisomerization of n-heptane. Process designs and operating plants for the hydroisomerization of pentane/hexane (C5/C6) do exist [16]. Because the reaction mechanism of the hydroisomerization of n-heptane is similar to that of C5/C6, the optional processes for the n-heptane isomerization are the existing C5/C6 isomerization processes, which can be classified into [15]:

I. Processes using $HCl/AlCl_3$ as a monofunctional catalyst
II. Processes using a noble metal on a chlorided alumina as a bifunctional catalyst
III. Processes using a noble metal on amorphous silica-alumina as a bifunctional catalyst
IV. Processes using a noble metal on a acid form of a zeolite as a bifunctional catalyst

Some process options for C5/C6 processes are given in Table 3-1[9].

Table 3-1. Process Options for the Hydroisomerization of C5/C6

Process name	Hysomer Process	BP Isomerization Process	TIP	UOP/Penex	IFP
Process type	IV	II	IV	II	IV
Company	Shell, UOP	British Petroleum	Shell, Union Carbide	UOP	ABB, Akzo Nobel
Date developed	1960	1965	1975	1950	
Type	Once through	Recycle	Recycle	Recycle	Recycle
Temp [°C]	250	100-150	240-260	120-170	250
Pressure [bar]	10-30	20-65	10	20-65	10
Catalyst	Pt/HMOR Zeolite	Pt/Cl-alumina based	Pt/HMOR Zeolite	Pt/Cl-alumina based	Pt Zeolite IS632
Pre-treatment	No	Yes	No	Yes	No
RON feed	73	72.2	na	70	na
RON product stream	82.1	84.6	90.7	84-85	80
Yield product (C5+) [w%]	97-98	99	>95	98-99	na
Capacity [t/d]	1,000	na	na	1,200	600

3.2.2 Process concept chosen

The reaction section of present hydroisomerization processes (C5/C6) generally consists of one reactor, where isomerization occurs, in the reaction section. In this conceptual process design the reaction section will contain two reactors:

- the first reactor where the reaction of n-heptane to mono- and dibranched isomers occurs
- the second reactor where the reaction of specific dibranched heptane isomer (2,4 DMP) to tribranched isomer (2,2,3 TMB) occurs. (See Appendix 25)

It is necessary to separate the reaction section into 2 reactors, because the sequential reactions (n-heptane → monobranched+dibranched isomer → tribranched isomer) require different acid strengths of the catalyst. If the catalyst is too acidic, cracking of dibranched alkanes is enhanced, which is undesired. If the catalyst is a too weak acid the isomerization reaction does not proceed appropriately (see reaction kinetics). The optimal solution is to operate the reaction section in 2 reactors.

The largest portion of the feedstock is C6, C7 and C8 alkanes. These fractions are n-alkanes, isoalkanes and cycloalkanes. To separate the C7 fraction from the lighter and heavier components use is made of two distillation columns, a tailing and a topping column. The preferable feedstock should not contain water and hydrogensulfide because these will poison the catalysts.
To separate the C7 fraction into a fraction, which is destined for the first reactor also a distillation column is used. The bottom fraction goes to the first reactor, while the topstream goes to the product separation membrane. This membrane separates the top stream into the product and a reactant stream destined for the second reactor.
The outlet of both reactors are both mixed and led to a hydrogen separation membrane. The recycle is then led through the topping distillation column.

Feed Capacity
It is assumed that the throughput of the feedstock is 1000 English tons/day, which is 907 metric t/d, thus 317450 t/a, assuming one year has 350 operating days. The assumption is based on the throughput of the existing C5/C6 isomerization processes, which varies between 600 and 1,200 t/d. See Table 3-1. With all other tons mentioned further in the report, metric tons (equal to 1000 kg) is meant.

Product Specifications
The objective of the n-heptane hydroisomerization process is to enhance the octane number (RON) of the feed. Since the product (isomerized n-heptane) will be used for the gasoline blending, the RON specification of gasoline is used for our product (see Table 3-2).

Table 3-2: Product Specifications of "regular grade"[17]

Property	Value
RON	90-95

The products of the plant will be a mixture with the highest possible octane number (RON) and will contain the following components: 2,2,3-TMB, 2,2-DMP and 3,3-DMP and a trace of
X 2,4-DM~~H~~x. P

Stoichiometry
There are two classes of reactions occurring during the isomerization of the n-heptane:

- Hydroisomerization: reaction of saturated alkanes to saturated iso-alkanes in the presence of hydrogen and a catalyst.
- Cracking: reaction of saturated alkanes to smaller alkanes in the presence of hydrogen and a catalyst.

The complete sets of stoichiometric reactions are presented in Appendix 23.

Reaction Kinetics
Acid-catalyzed skeletal isomerization of alkanes occurs via carbenium ions as intermediates [15]. The isomerization reaction itself is part of a chain reaction, i.e. reaction cycle involving chain initiation, carbenium ion arrangement and chain propagation.

It is assumed that all isomerization and cracking reactions taking place follow first order kinetics. The most likely mechanism of skeletal isomerization of the intermediate carbenium ion involves the rearrangement of the classical secondary carbenium ion into a nonclassical carbonium ion, namely a protonated dialkylcyclopropane (PCP) as suggested by Sie [15]. Since cracking and isomerization are both catalyzed by similar acid catalysts, it is plausible that cracking may occur alongside isomerization, thus decreasing isomerization selectivity. Cracking is found to be consecutive to isomerization [11].

A list of the complete stoichiometric reactions is inAppendix 23: Stoichiometric reactions. Due to the complexity of the calculations and the limited amount of kinetic data available, reacting species may be lumped to isomer groups in which the individual species are at thermodynamic equilibrium. In chapter 8 a full description of the fit of the reaction kinetics is given.

3.2.3 Catalysts

In principle, there are two types of catalysts for skeletal isomerization of paraffins via carbenium or carbonium ions as intermediates [15]: monofunctional acidic catalysts and bifunctional catalysts that combine the acidic function with the hydrogenation-dehydrogenation function of a metal.

For this process there are 2 catalysts chosen:

- In the first reaction unit, where n-heptane reacts to mono- and dibranched isomers, the strong-acidic zeolite-based Pt/Hbeta with 0.5 w% Pt will be used as a (bifunctional) catalyst. This catalyst was chosen, because it had the highest conversion and selectivity to isomerization, and thus the least cracking (see Appendix 25)
- In the second reaction unit, where only certain dibranched isomers react to tribranched isomer (2,2,3 TMB), the medium/weak-acidic amorphous silica/alumina with 5 w% Ni will be used as catalyst. This catalyst is chosen because it was the only catalyst where some experimental data was available, and it was specifically tested for the conversion of dibranched to tribranched molecules.

A summary of the catalyst properties of the chosen catalysts is in Table 3-3.

Table 3-3: Catalyst Properties

		Reactor 1 Reaction: n-heptane → monobranched + dibranched	Reactor 2 Reaction: dibranched → tribranched
Catalyst type		Zeolite Hbeta	Amorphous Silica/alumina
metal loading	[w%]	Pt 0.5	Ni 0.5
Si/Al ratio	[-]	10.8	n.a.
Shape		Spheres	Spheres
Particle diameter	[mm]	3	1
Void fraction	[-]	0.5	0.5
Lifetime	[yrs]	2	2

3.2.4 Separations

The feedstock is separated into the desired reactants and products with distillation columns. The first separation column separates the heavy components (≥C8) from the C6 and C7 fraction. In the second distillation column the recycle and the distillate of the first column is separated into a light fraction (≤C6) and a C7 fraction.

The third distillation column separates the linear and monobranched isomers from the multibranched isomers.

In the first membrane the multibranched isomers are separated by size exclusion (see Table 3-4 and Table 3-5), this means that only 2,2-DMP, 3,3-DMP and 2,2,3-TMB are excluded by the membrane and all other components will flow to the second reactor. It is assumed that all components with a kinetic diameter than 5.5 Å will flow through the membrane. The separation is 100 %.
The hydrogen will be separated from the outlet stream from both reactors by a membrane. The data for H_2 is in [21], see Table 3-6.

As can be seen from Table 3-4, isomer separation by distillation is rather difficult. However, separation by size exclusion is possible using a molecular sieve membrane.

Table 3-4: Kinetic Diameter and Boiling Point of n-Heptane and its Isomers

Molecule		Boiling point (°C)	Kinetic diameter (Å)
n-heptane	n-C7	98.5	4.2
2-methylhexane	2-MHx	90.0	5.0
3-methylhexane	3-MHx	92.0	5.0
3-ethylpentane	3-EP	93.5	5.0
2,3-dimethylpentane	2,3-DMP	89.7	5.0
2,4-dimethylpentane	2,4-DMP	80.4	5.0
2,2-dimethylpentane	2,2-DMP	79.2	6.0
3,3-dimethylpentane	3,3-DMP	86.0	6.0
2,2,3-trimethylbutane	2,2,3-TMB	80.8	6.0

The following data (Table 3-5) on the separation of C6-C8 isomers using zeolitic membranes are available in the open literature. The permeance is the mole or mass flux through the membrane per time per pressure difference. The selectivity, $\alpha_{i,j}$, is defined as ratio of the molefractions of the components i and j in the feed and permeate.

Table 3-5: Membrane Data for Size Exclusion Separation

Zeolite type	Size (Å)	Chain	T (K)	Permeance mol/m^{2}sPa	Selectivity (Permeate/ retentate)	Reference
Silicalite	5.4	n-C6	423	$1\cdot10^{-7}$		Funke [5]
Silicalite	5.4	n-C8	410	$1.2\cdot10^{-7}$	40	Funke [5]
Silicalite	5.4	n-C6	373	$6\cdot10^{-8}$	50	Vroon [18]
Silicalite	5.4	n-C7	374		30‡	Schenk [14]
ZSM-5	**5.4**	**n-C6**	**400**	**$1\cdot10^{-7}$ ($1\cdot10^{-8}$)***	**1000 (35)***	**Flanders [4]**
ZSM-5	5.4	n-C6	373	$1\cdot10^{-7}$	250	Krishna [6]
ZSM-5	5.4	n-C6	373	$1\cdot10^{-7}$	1000	Coronas [2]
MFI (ZSM-5)	5.4	n-C6	303	$1.4\cdot10^{-9}$*, $1\cdot10^{-9}$†	130*, 50†	Matsufuji [10]
ITQ-1	5.5	n-C7	450		15‡	Corma [1]
MCM-22	5.5	n-C7	650	$28\cdot10^{-6}$	8.7‡	Sastre [13]

* Liquid phase (pervaporation)
† Liquid phase mixture with 2-methylpentane
‡ Molecular dynamics simulation

As can be seen, 5.5Å zeolites have been effectively applied in research studies, as their fairly large pores allow the highest diffusion speeds, and yet induce acceptable separation selectivity.

There is no (satisfying) literature about C7 hydrocarbons, so literature about C6 is used and it is assumed that the C7 linear and branched hydrocarbons behave the same as the C6 linear and branched hydrocarbons. The membrane of Flanders [4] is chosen, because of high selectivity and permeance.

The membrane separation is done by pervaporation. In pervaporation, the driving force is the difference in partial pressure on the gas side and the vapor pressure on the liquid side of the membrane. The advantage of pervaporation over gas permeation is that higher fluxes can be established when the component that needs to be removed from the liquid stream has a relatively high activity, i.e. even at low concentrations it has a strong tendency to evaporate. To obtain the best performance the high pressure side of the membrane will be operated in the liquid phase (10 bar) and the low pressure side in the vapor phase (1 bar). A sweep gas will be used on the permeate side. The basic setup for a reactor-membrane section is show in Figure 3-1:

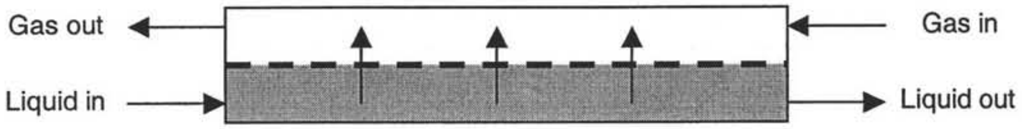

Figure 3-1: Basic Design Concept Membrane Section

Hydrogen is separated from the first reactor effluent with a membrane. The data used for the hydrogen recovery membrane is given in Table 3-6.

Table 3-6. Hydrogen membrane data

Zeolite type	Size [Å]	T [K]	Permeance [$m^3(STP)/m^2.h.bar$]	Selectivity	Reference
ZSM-5	5.4	473	$1\cdot10^{-7}$ $(1\cdot10^{-8})^*$	>> 500	de Vos and Verweij [21]

3.2.5 *Block Schemes*

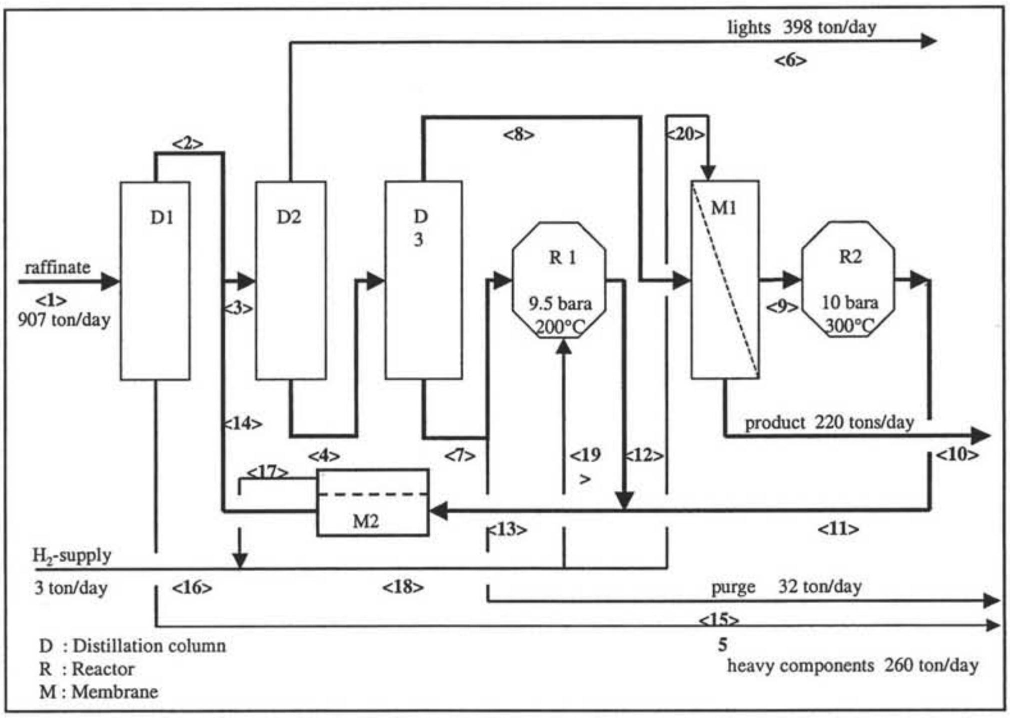

Figure 3-2: Block Scheme (simplified) for the Hydroisomerization process of n-Heptane

All the in- and outgoing streams of block scheme Figure 3-2, are summarized in Table 3-7.

Table 3-7. Stream summary

Stream number	Stream description	Mass flow [ton/day]	Yield [t/t product]
1	HC feed, raffinate	907	4.12
16	Hydrogen make up	3	0.014
10	product	220	1
6	light components	398	1.81
5	heavy components	260	1.18
15	purge	32	0.15
14	recycle	2521	11.5
17	Hydrogen recycle	328	1.5

A complete stream summary per component can be found in Appendix 2.

3.2.6 Thermodynamic Properties

For the hydroisomerization process the Aspen Plus User Guide suggests the use of the thermodynamic models by Chao-Seader (CS), Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK). As a general model RKA is used.
The thermodynamic equilibrium composition of n-heptane and the n-heptane isomers are calculated in Aspen Plus 10.0. The result is graphically presented in Figure 3-3.

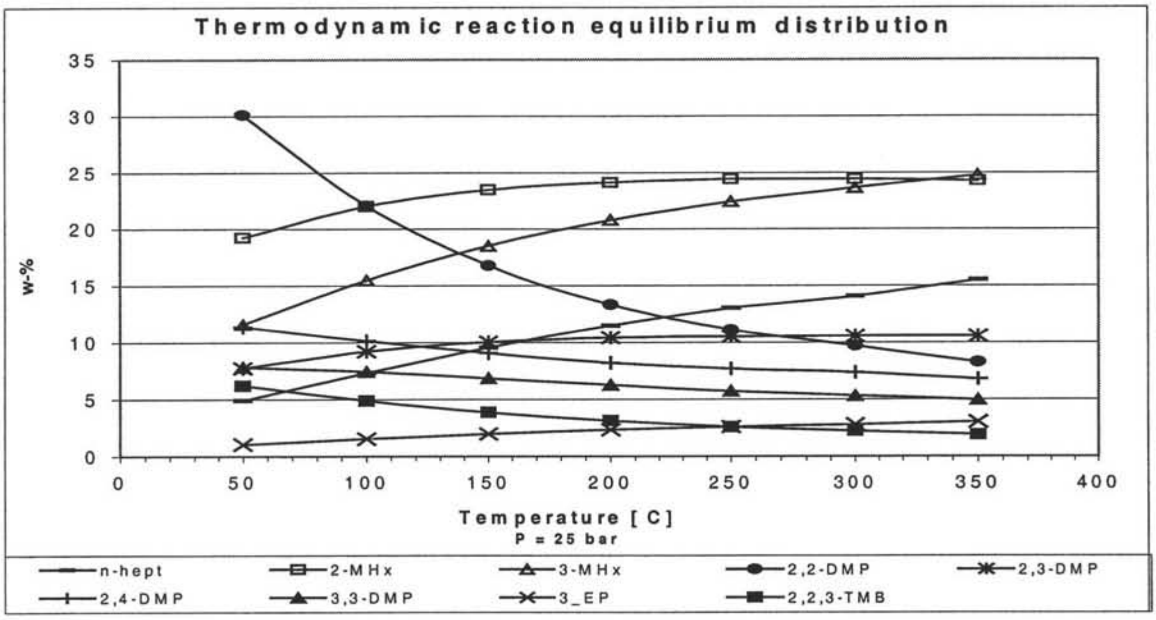

Figure 3-3: Thermodynamic Equilibrium Distribution of n-Heptane Isomers at 25 bar (data calculated in Aspen Plus 10.0)

At lower temperature, more 2,2,3-TMB will be formed. However the temperature must be high enough for a sufficient conversion.

Figure 3-4 shows the temperature dependency of the product octane number (RON). It can be seen that if only the high-RON products are withdrawn from the reaction mixture, the temperature dependency is small. The RON numbers are calculated with the following formula

$$Ron_{mixture} = \sum_{i} x_i \cdot Ron_i \tag{3.1}$$

The RON of each component is given in Appendix 24.

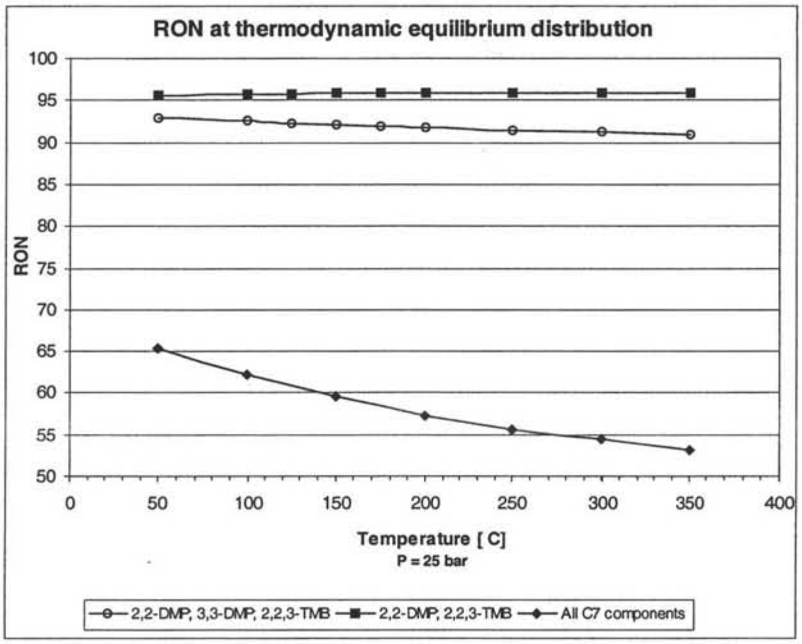

Figure 3-4: Octane Numbers of Equilibrium Mixture as Function of Temperature

3.2.7 List of Pure Component Properties

A list of pure component properties is provided in Appendix 24. The table contains all components with their systematic names, formula's, molecular weights, RON, densities, boiling point, melting point and where available the MAC and LD_{50} values.

3.3 BASIC ASSUMPTIONS

3.3.1 Plant Capacity

The plant will process a feed of 907 t/d. All the in- and outgoing streams are defined in name and quantity in the block scheme in Figure 3-2.

3.3.2 Location

The plant will be located in Europoort, Rotterdam in the Netherlands.

3.3.3 Battery Limits

The battery limits for the conceptual process design is shown in Figure 3-5. It is assumed that the feed has a composition as mentioned in Appendix 2, 6 and 7.

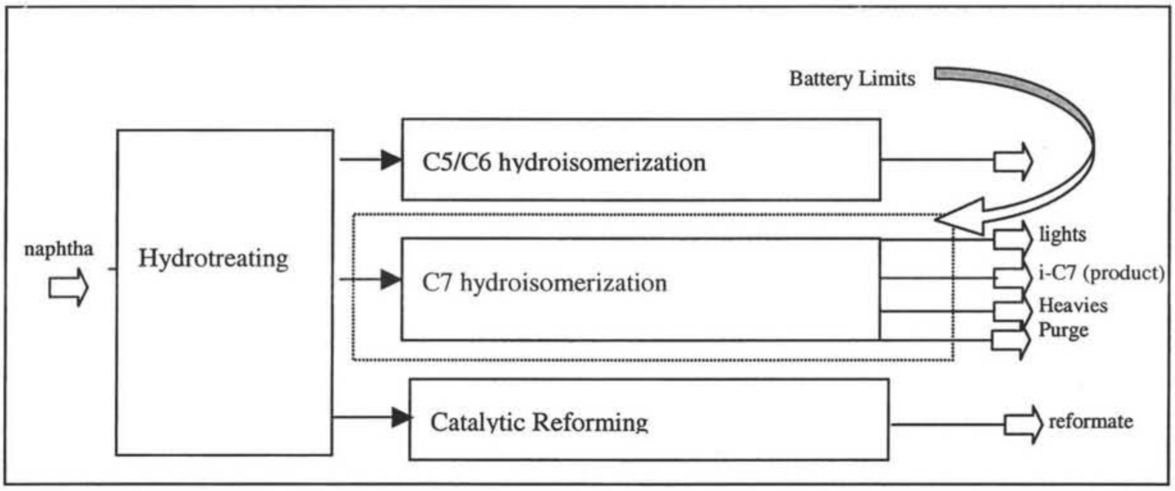

Figure 3-5: Proposed Battery Limits for the Hydroisomerization of n-Heptane (CPD 3259 project)

3.3.4 Definition of All In- and Outgoing Streams of Battery Limits

All the in- and outgoing streams per component are summarized in Appendix 2, 6 and 7. Also a summary of the mass streams is shown in Table 3-7.

Feed

The following assumptions are made:

- The n-heptane-rich feed, traditionally going to the catalytic reformer, is coming from the naphtha hydrotreater on the site
- All components with a boiling temperature 20°C higher than n-C7 are neglected
- All components less than 0.5 wt % are neglected
- All other cyclic compounds are neglected, due to the unknown behaviour in the reactors
- The feed has less than 10 ppm water content
- The feed has less than 20 ppm sulfur content
- The feed has a RON of 56.7 [19]
- The hydrogen is supplied on-site, without any problems. Hydrogen make-up is added to increase the pressure and facilitate the hydrogenation-dehydrogenation on the catalyst. Unfortunately, hydrogen is also consumed in small amounts due to cracking.

Products

The composition of the product can be found in Appendix 7.

- The product (isomerizised heptane) will be sent to a gasoline blending unit (outside the battery limit) where it will be added to the gasoline pool
- The lights (mostly butanes and propane) will be used outside the battery limits as fuel, but can alternatively also be used within battery limits
- The heavies, which contain mostly octanes and heavier components, will be sent to the catalytic reformer. These heavies have a higher RON than the feed.

Utilities

It is assumed that the utilities are available on the plant site and they are listed in Appendix 26.

3.4 ECONOMICS

3.4.1 Maximum Allowable Investment

The following assumptions are made:

- The price of the feed, the product, the purge, and the heavy components are based on the price of Light Straight Run Naphtha (Light SRN), 362.08 fl/t [12]
- The price of the light components (mostly propane and butane) is calculated based on the gross heat value
- The price of the other by-products ("Heavy Components" and "Outlet Reactor 2" is assumed to be dependent on their RON number see Appendix 19.

The calculations for the economic margin are summarized in Table 3-8

Table 3-8: Economic Margin

Stream	**Battery Limit IN/OUT**	**Mass Flow** t/d	**Price** fl/t	**Total price**[1] Mfl/a
Straight Run Naphtha (C7-rich stream)	IN	907.2	362.08 [2]	115.0
H_2 Make-Up	IN	3.1	2,000 [3]	2.2
Subtotal				**117.2**
Product isomerized C7 stream	OUT	220.4	1035.07 [6]	79.8
Light Components (≤C6)	OUT	397.6	315.97 [5]	44.0
Heavy components (≥C8)	OUT	260.4	852.05 [6]	77.7
Purge	OUT	31.9	55.13 [6]	0.6
Subtotal				**202.1**
Margin				**84.9**

[1] It is assumed that 1 year has 350 operating days

[2] Source [12] and [19]

[3] Source ir. C.P.Luteijn

[4] Assumed the same as the gasoline price minus the taxes

[5] Assumed the same as the fuel value times the natural gas price

[6] Estimated by its RON-number

To calculate the maximum allowable investment a discount cash-flow analysis was made according to [**3**]. The plant life is assumed to be 10 years and there is a 2-year start-up period. The results are depicted in table 3-9.

Table 3-9. Maximum Allowable Investment at an interest rate of 10%

Year	NCF Mfl/a	NFW Mfl/a	DCF @ DCFROR 10% Mfl/a	Accumulative DCF Mfl/a
1		0.0	0.00	0.0
2		0.0	0.00	0.0
3	84.90	84.9	63.79	63.8
4	84.90	169.8	57.99	121.8
5	84.90	254.7	52.72	174.5
6	84.90	339.6	47.92	222.4
7	84.90	424.5	43.57	266.0
8	84.90	509.4	39.61	305.6
9	84.90	594.3	36.01	341.6
10	84.90	679.2	32.73	374.3
11	84.90	764.1	29.76	404.1
12	84.90	849.0	27.05	431.1
Total			431.1	

3.4.2 Sensitivity analysis

To check the influence of price changes in the feed and the product, at an interest rate of 10 %, a sensitivity analysis is made and shown in Table 3-10.

Table 3-10: Sensitivity Analysis

In the sensitivity the operating costs and the total investment is taken into account. At a product price increase of at least 6.4 %, the plant will be profitable.

Variation %	**Operational costs** Mfl/a	**Income** Mfl/a	**Margin** Mfl/a	**Max. investment** Mfl/a	**Calculated investment** Mfl/a
Variation Feed price					
-15	178.99	202.09	23.10	117.3	88.59
-10	185.14	202.09	16.95	86.1	88.59
-5	191.29	202.09	10.80	54.8	88.59
0	197.44	202.09	4.65	23.6	88.59
5	203.59	202.09	-1.50	-7.6	88.59
Variation Product price					
-10	197.44	181.9	-15.54	-79	88.59
-5	197.44	192	-5.44	-27.7	88.59
0	197.44	202.09	4.65	23.6	88.59
5	197.44	212.19	14.75	74.9	88.59
6.4	197.44	215	17.56	89.3	88.59
10	197.44	222.3	24.86	126.2	88.59

4. THERMODYNAMIC PROPERTIES

The model to compute thermodynamic and transport properties was chosen, based on the criteria in the Aspen Plus guide. Recommended models were Peng-Robinson (PR), Soave-Redlich-Kwong (SRK) and Soave-Redlich-Aspen (SRA).
These models perform well in petroleum refinery processes. Normally all three models will give about the same results, except in cases where there are close boiling components in the system, as in our case. In that case it is better not to choose PR or SRK, because the PR-equation and the SRK equation predict the boiling temperatures not as precise than Redlich-Kwong-Aspen RKA. Therefore RKA is the general model in the present work. [9]

The Redlich-Kwong-Aspen equation-of-state is the basis for the RK-ASPEN property method. It can be used for hydrocarbon processing applications. It is also used for more polar components and mixtures of hydrocarbons, and for light gases at medium to high pressures.

The isomerization reaction is equilibrium limited. As can be seen in the thermodynamic equilibrium graphs, which are shown in Figure 3-3, a low reaction temperature favors isomerization to 2,2,3-TMB.

The T-xy plots of the key components of the three distillation columns are shown in Appendix 4. These show that there are no irregularities or inconsistencies, therefore they seem reliable. Also no difficulties like azeotropes are present in the separations. In Appendix 5 the thermodynamic properties of all relevant components are given. The dependency of the heat capacity of the components for the liquid and the gas state is given. Also the Antoine constants for the calculation of the vapor pressure is shown.

A comparison between the Aspen data and literature data is made. It seems that most Aspen data is comparable with the literature data, but the Gibbs free energy of formation is quite different. Also the specific heat that is used in Aspen differs max. 13 % from the literature data. Despite this difference, this data was used for the simulations.

5. PROCESS STRUCTURE & DESCRIPTION

In the foregoing chapters, the process has been formulated. The specific design criteria and their motivation are given in chapter 2 and chapter 3. Any details about the selected unit operations and process will be revealed in this chapter.

5.1 CRITERIA AND SELECTIONS

A detailed description on process criteria and selections is given below.

5.1.1 Distillation Columns

Tailing column (C01)

C01 is a column that separates the heavy components (C8 and higher) from the light components (C6 and C7). The key components are n-C7 and 2,4DMHx, because the difference in boiling temperature is ca. 10 K. The separation is atmospheric for safety reasons. A low pressure is preferable because the separation is better at lower pressure. Choosing a distillation under vacuum conditions is not desirable because in cases of accidents, like a leak, the column will be filled with air, which can cause explosions or other kind of damages. Therefore a distillation under atmospheric conditions will cause less serious problems in cases of leaks. The design specifications for top and bottom are set at such a value that the column is not too large and a sufficient amount of product is produced. The condenser is a partial condenser. Reboilers are described below.

Topping column (C02)

In this column the fraction C6 and lighter components is separated from the C7 fraction. The feed is the top stream from C01 and the recyclestream. The same explanation for the pressure and design specifications as for C01 applies to this column. The condenser is a partial condenser.

Reactant separation column (C03)

This column separates the feed for R01 (linear and monobranched C7) from the feed to M01. This column operates under atmospheric conditions for the same reason given in the section above D01. Because the feed to the membrane needs to be liquid, a total condenser is used.

Reboilers for C01, C02 and C03

It is assumed that there is enough headroom available for reboilers outside the column. Forced circulation reboilers are not required as we are not dealing with viscous and heavily fouling process fluids. As kettle reboilers have lower heat transfer coefficients than the other types, vertical thermosyphon reboilers are chosen. The distillation operation occurs at normal pressure (between 1 and 1.4 bara). It should be noted that the thermosyphon reboiler should be constructed at an elevated base to provide the hydrostatic head required for the thermosyphon effect.

Condensors for C01, C02 and C03

There are no extreme temperature differences between shell and tube side and the pressure on both shell and tube-side is about 1 bara. Fixed tube, one pass shell (E shell) is chosen as this is the simplest and cheapest shell and tube exchanger. Air cooling is not a good option because the condensation temperature is too low, therefore water cooling is applied.

5.1.2 Reactors

Reactor for conversion of n-heptane and mono-isomers (R01)

The isomerization reactor is a fixed packed bed reactor with interstage cooling. The interstage cooling is used to keep the temperature constant. The catalyst is a Pt-Hbeta zeolite with 0.5 wt % platina, which is thermally stable. The reactor is operated at 473 K, since deviation from the experimental results would give uncertainties, because little is known about the behaviour of the catalyst at varying temperatures. Hydrogen is present in the reactor, in the same ratio as described in the literature, as a cocatalyst and to avoid cracking. n-Heptane is converted to monomethyl-isomers and the monomethyl-isomers are converted to the dimethyl-isomers. The reactor is optimized to produce as much 2,4-DMP as possible.

Reactor for conversion of 2,4-DMP (R02)

The second isomerization reactor is an adiabatic fixed packed bed reactor.
The used catalyst is alumina silica with 5 wt % nickel. No other details, but conversion, about this catalyst are known. For this reason and the above-described reason, the temperature in the reactor and the amount of hydrogen is the same as in the literature.
In the reactor 2,4-DMP is converted to 2,2,3-TMB. [29]

5.1.3 Membranes

Product separation membrane (M01)

The membrane is a ZSM-5 layer of 10 micrometer supported on a alumina. [4] The membrane is a cross-flow monolith. Since this geometry only provides unit dimensions that can be realized in practice (e.g. shell&tube units would be too large to build). This membrane is very large, which is caused by slow permeation of the components. The membrane is based on pervaporation, and this method of operation gives the best performance. The necessary surface is 20,000 m^2. Smaller membranes are possible when the membrane thickness can be reduced. Another kind of membrane is also possible, when activated gas diffusion is possible. All phases are gases then, but the speed of separation is much faster. Unfortunately no data was available in the literature about activation energies of the relevant components.
Assumed is that all components smaller than 5.5Å pass trough the membrane and the membrane is ten times thinner than the literature membrane. [4]

Hydrogen separation membrane (M02)

Use is made of a membrane that is made with a Sol-Gel preparation method. Therefore the membrane thickness can be very thin, 30nm, which cause a faster permeation in comparison with traditional preparation methods. The necessary surface area is 4,000 m^2. The membrane is made of amorphous silica. The pore size diameter is found to be 5 nm. The separation was very good, since all longer alkanes other than methane were completely excluded. Use is made from a cross flow monolith membrane. [21] Assumed is that only hydrogen passes through the membrane.

5.2 PROCESS FLOW SCHEME

A detailed process diagram is presented in Appendix 1.

5.3 PROCESS STREAM SUMMARY

The process stream summary is shown in Appendix 2.

5.4 UTILITIES

A summary of all available utilities can be found in Appendix 26, while the used utilities are in Appendix 9.

5.5 PROCESS YIELDS

Process flows and process yields are summarized in Appendix 10. A comprehensive block scheme of the in- and out going streams is also provided.

6. PROCESS CONTROL

The aim of process control is to reduce the variability of the process. This is to ensure safe plant operation, a controlled production rate and a standard product quality, while keeping the operability costs as low as possible. To achieve this, the plant is equipped with instruments to monitor and control the key variables during plant operation. The control system is shown in the process flow diagram in Appendix 1. [9]

6.1 KEY VARIABLES

The following criteria are used to place the control devices in the scheme:

- Identify which control loops are needed for a steady state operation, such as level, flow, pressure and temperature controls
- Identify the key process variable that needs to be controlled to achieve the specified product quality

6.2 CONTROLLERS FOR EACH PROCESS UNIT

6.2.1 Feed, recycle and purge streams

Feed

The feed is designed to be 907.18 t/d, which is accomplished by the flow sensor connected with a control valve in the feed.

Recycle stream 49

A flow control valve controls the flow of the recycle stream. A flow controller is chosen, because the dimensions of the units limit the recycle stream, and large fluctuations in recycle flow rate cause major disturbances in process operation.

Purge stream 39

After P06 a purge is controlled with a pressure controller, which is the only pressure controller for the R01 section. The pressure sensor is connected with a control valve in stream 39.

H_2 purge stream 52 and 53

The purge is present for safety reasons, however in the design all hydrogen is recycled and the control valve is default closed. So only when a pressure increase is measured in stream 52, the valve will release the excess pressure to prevent accumulation of impurities in the recycle loop.

6.2.2 Distillation Columns

Distillation column C01

The objective for control is to operate the distillation column safely; this means that overflows or dry up of the column will be prevented. The quality of separation is not controlled directly.

In the top of the column a pressure sensor is present. This sensor also controls compressor K01. In stream 6 a temperature sensor is available which interacts with the cooling water flow. Also a level sensor in V01 is present, which is connected with a control valve that controls the reflux flow.

In the bottom section two control loops are present. The first is the temperature sensor, which is connected with the steam flow. When the temperature decreases in the bottom the flow of the steam will be increased.

The other control loop is a level controller in the bottom, which is connected with the control valve of the outgoing stream.

Distillation column C02
The bottom section is in the same manner controlled as C01, in the top only the pressure control differs. The pressure control is connected with a control valve instead of a compressor.

Distillation column C03
Also this column has the same bottom control and the control of the top is different.
The reflux, stream 27, is kept constant with a flow controller. The level in V03 is kept constant with a control valve in the distillate stream, stream 27.

6.2.3 Reactors

Reactor 1 R01
The temperature of the reactor must remain in a temperature range, otherwise product selectivity would decrease due to enhanced cracking reactions. The temperature of the reactor is controlled by interstage cooling.
The temperature controller of E07 is connected with a temperature sensor in the reactor inlet.
The temperature controller of E08 is connected with a temperature sensor before the second catalyst bed. The temperature controller of E09 is connected with a temperature sensor before the third catalyst bed. Also the ratio between hydrogen and the hydrocarbon stream must be controlled.
The hydrogen that is supplied, stream 56, depends on stream 41. Therefore a flow indicator in 41 is connected with a ratio flow controller. The ratio flow controller controls the duty of K02.

Reactor 2 R02
The objective to be controlled for R02 is the temperature of the inlet flow. The temperature controller controls the heat duty of F01. The pressure in R02 is slightly higher than R02 and is controlled by a control valve in stream 35. The hydrogen supply depends on the incoming hydrocarbon stream (stream 29). A flow indicator is connected with a ratio flow controller, which controls the duty of K03.

6.2.4 Membranes

Product separation membrane M01
The membrane is operated at a specific temperature at feed side. The temperature of the membrane inlet is controlled in E10. A temperature sensor is therefore connected with the steam flow from E10. The product stream is led through a control valve, which is in connection with a pressure sensor, to ensure a specific pressure in the membrane unit.
A pressure sensor at the permeate stream is used to control the compressor duty of K03, to ensure a constant pressure at the permeate side.

Hydrogen separation membrane M02
Objective is to operate M02 at a specific pressure at the feed side and to ensure enough make-up hydrogen on the permeate side. On the feed side the pressure is controlled with the pressure sensor connected with a valve in stream 39. In stream 50, H2-make-upstream, a flow sensor is connected with a control valve, to ensure the flow of hydrogen at the permeate side. The pressure is controlled by the control valve in stream 59 (H_2 purge).

6.2.5 Furnace

A temperature controller in the outgoing stream controls the furnace. This time controller is connected with the inlet flow of air and fuel.

6.2.6 Heat exchangers

A temperature sensor in the outgoing stream is connected with the flow controller of the cooling water or steam.

7. MASS AND HEAT BALANCES

In this chapter mass and heat balances over the process will be discussed. A mass and heat balance will be made over the battery limits and over the equipment. In theory no differences in total mass and energy of the in- and outgoing streams may exist.

7.1 BALANCE OVER THE BATTERY LIMIT

Table 7-1. Mass and heat balance over the battery limit

Streams in	Mass flow [tonne/day]	Enthalpy [KW]	Streams out	Mass flow [Tonne/day]	Enthalpy [kW]
1	907.18	-20081	4	260.35	-5981
31	3.12	-19.6	18	397.62	-9612
			31	220.44	-4413.02
			40	31.89	-778
Total	910.30	-20100.6	Total	910.30	-20784

Table 7-2. Deviations in mass and heat flows

	Amount	
Mass flow	$2.2 \cdot 10^{-5}$	tonne/day
Heat flow	-683	kW

The mass balance inequality is very small, it's about 8 kg/a on a total amount of 43200 tonne/a. This deviation is total dependent on the tolerance that's used in Aspen.
The heat balance shows that about 683 kW has to be withdrawn from the process. This amount should be equal to the amount, which is withdrawn by the equipment. In Appendix 8 the mass and heat summary over the equipment is given. The mass balance over the equipment inequality is also in this case very small. The heat that is withdrawn from the streams by the equipment is 683 kW. The deviation of the heat balance is therefore 0 kW. In Appendix 7 a component balance is given which also shows the enthalpy of -683 kW. It can therefore be concluded, that the mass and heat balances satisfy the theory that no deviations may exist between the in- and outgoing streams.

7.2 PINCH TECHNOLOGY

In this chapter the possibility of pinch technology is examined. The technology is totally based on the method described in. [24] First a summary is given for the selected cold and hot streams in Table 7-3. Then the data of these streams are given in Table 7-4.

Table 7-3. Summary of available hot and cold streams

Streams	Utility
Hot stream	Cooling
55	E11
Cold streams	Heating
41	E07
28	E10

Table 7-4. Data for heat integrating problem.

		Cold		Hot
Equipment		E07	E10	E13
Heat duty	[kW]	9700	3800	-4558
Cp	[kW/K]	91.9	38.8	42.3
Cp	[kJ/kg.K]	2.6	2.9	14.5
T0	[K]	367	360	504
T1	[K]	473	458	396

Adding the heat capacities of the streams makes the cold composite. Since there is only one hot stream, no hot composite graph is made. The cold composite is given in Figure 7-1.

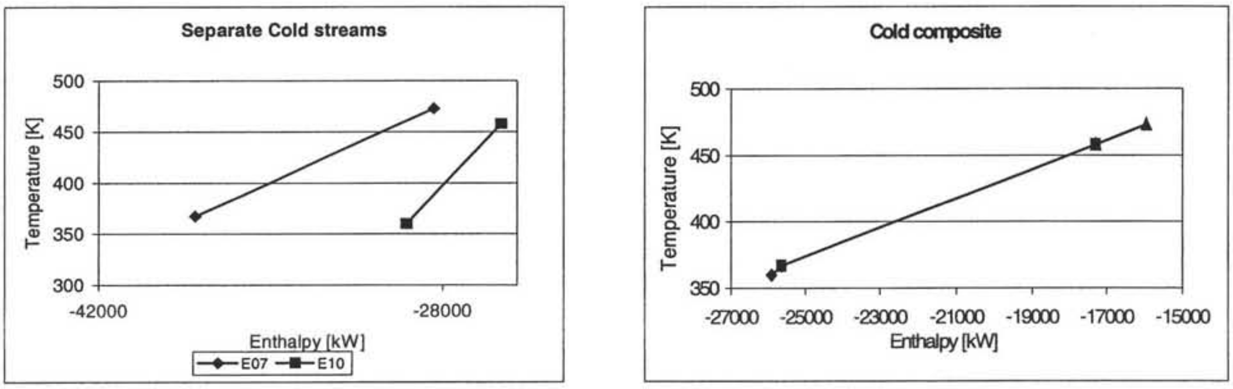

Figure 7-1. Separate cold streams and composite of cold streams

The cold and hot composite is given below. A minimum temperature difference is taken at 10 K (as recommended by [24]), since the target temperature of the hot stream is 396 K the pinch temperature is 386 K.

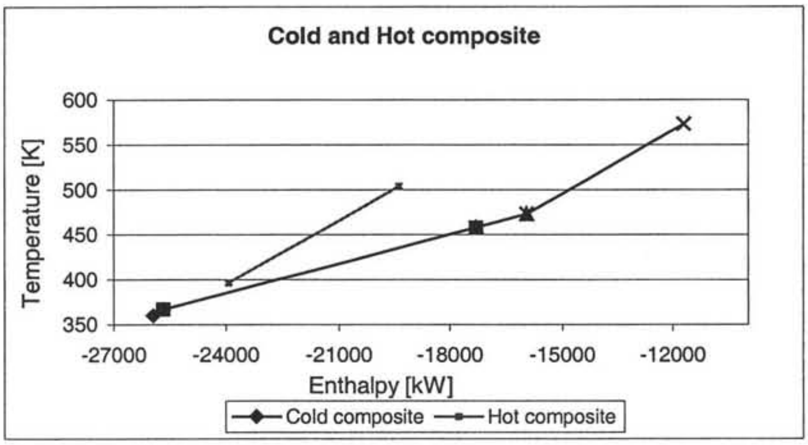

Figure 7-2. Hot and cold stream composite curves

Following the rules in [24], working above the pinch temperature is only possible when $C_{p,hot} \leq C_{p,cold}$, and below pinch temperature $C_{p,hot} \geq C_{p,cold}$, these rules most be obeyed otherwise the minimum temperature difference would be violated. This means for our streams that working above pinch temperature is possible when stream 55 is coupled with stream 33. However this isn't a very smart choice, because stream 33 can be only partially heated up by stream 28, while stream 28 cannot be cooled totally by stream 33.

Another possibility is coupling stream 55 with stream 28, because this stream 28 can be entirely heated up with stream 55. A pinch temperature is not the case here, since the minimum temperature difference is 46 K.

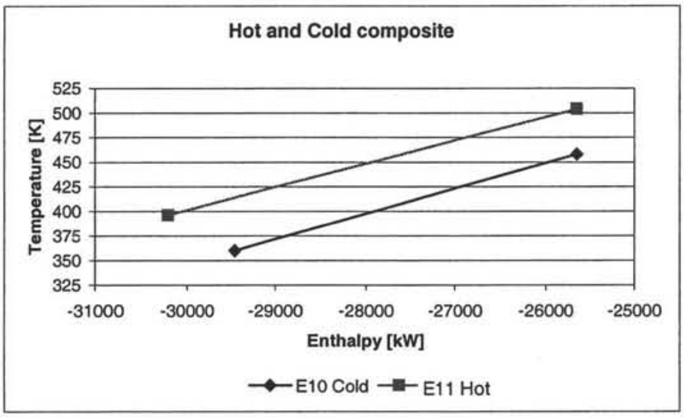

Figure 7-3. Hot and cold streams of E10 (stream 28) and E13 (stream 55)

Stream 28 from E13 will not be cooled entirely. The remaining cooling duty of the cooler is now only –758 kW. This is 17 % of the original heat duty required for E11 (before applying pinch technology). Applying pinch technology will save 151.8 t/d HP steam (which was necessary for E10) and 3900 t/d cooling water.

This coupling will save 1.7 Mfl annually.

8. PROCESS AND EQUIPMENT DESIGN

In this chapter the process and equipment design will be discussed. Details are given on the process simulation and the background of the equipment sizing.

8.1 PROCESS SIMULATION

The designed process is simulated in the steady state flowsheet program ASPEN Plus 10.0-1. This program handles all equipment used in the design and calculates the mass balance and heat balance. The specific dimensions of all the equipment are calculated in Excel.

Aspen+ Simulation
The simulation is performed with the thermodynamic model Redlich-Kwong-Aspen, from which the argumentation is already discussed in chapter 4.

General assumptions:
- Reactions only take place in reactors, nowhere else
- Heat-loss in equipment and pipelines are not taken in account
- Pressure drops in pipelines are not taken into account

A more extended description of the simulation can be found in Appendix 11.

8.1.1 Feed composition

The feed is obtained from Shell [19]. It contains a wide range of compounds, from C5 to C11.
In order to make the feed more manageable for the CPD it will be simplified. First all the compounds which have a boiling temperature 20°C higher than n-heptane are neglected, because they will leave with the heavy compounds stream without any trouble. The total amount of these neglected compounds is 53.8 wt %. Also compounds which are in a smaller amount than 0.5 wt % present are neglected. This amount is in total 11.8 wt % of the original feed. Some cyclic compounds that are still present in the reduced feed are also neglected because nothing is known about their behavior in the reactors. This is 13.8 wt % of the original feed. The design feed contains by now only 20.6wt % of the original feed. This design feed and the original feed are in Appendix 6.

8.1.2 Distillation columns

The distillation towers are operated at 1 bara + pressure drop, because a better separation is obtainable at the lowest possible pressure, but for process safety it is better to work above atmospheric pressure. It is safer, because in case of a leak the content will stream out of the column, instead air streams in the column. A possible explosion in a column can cause much more damage than a explosion in the "open air". Recoveries are chosen to obtain the highest profit with the lowest costs. Costs are as well the number of stages and energy requirements. The profit is considered to be the largest product stream.

8.1.3 Reactors

The reaction kinetics described in Appendix 13 is used in the models.
The first reactor is operated at 473 K and 9.5 bara. The model used is an isothermal plug-flow reactor. The temperature is chosen to be near the experimental data. The calculations would be too inaccurate when the temperature changes. The optimal pressure is calculated by Aspen. To ensure a high 2,4-DMP yield, a small recycle stream, a small catalyst bed and a pressure that is

not too expensive to obtain. The recycle stream is directly related to the size of C02 and C03, a small recycle favors smaller columns.

The second reactor is operated at 573 K and 10 bara. The model used is an adiabatic plug-flow reactor. The temperature is chosen to be near the experimental data. The calculations would be too inaccurate when the temperature changes. Aspen calculates the pressure, to ensure a high 2,4-DMP yield in the first reactor and a high product yield in the second reactor, with a small recycle stream, a small catalyst bed and a pressure that is not too expensive to obtain.

Major problems exist with the cracking reactions. When one of the two reactors is set too small, ASPEN reports the following error: "reaction rate is set to zero, hydrogen is not present in reaction ...", even though hydrogen is present in extreme excess. Probably this error reflects a mathematical problem, because physically this message makes no sense.
To avoid this error, the simulation was started with a large reactor size and then decreases the reactor size with small steps. When the simulation has run with no errors, all other changes must be small in order too keep the errors out.

8.1.4 Membranes

The membranes are simulated with a simple component splitter, in Excel the real membranes are modeled.

8.1.5 Pumps and compressors

Pumps are needed to let the stream flow. Every stream is checked that is total liquid, since vapor causes extreme damage to the pump. A simple model is used for the calculation of the pump power. Compressors are needed to increase the pressure of the gas to obtain a gas flow.
The model is isentropic, because it's a common used model for industrial compressors [24]. K03 is a three-stage compressor because the pressure ratio is preferred to be below 3 bars per stage. [24]

8.1.6 Heat exchangers

Heat exchangers are modeled in Aspen, using estimates for the overall heat transfer coefficient U. Aspen calculates the optimal utility mass-flows and exchange area's, which should be minimalized.

8.2 EQUIPMENT DESIGN

8.2.1 Distillation columns

In this paragraph the procedure for designing the distillation columns is presented, as described by [24]. The operating range of a distillation column is set over a limited range of vapor and liquid flow rates. Flooding sets the upper limit of the vapor flow and can be caused by either carry over of liquid to the next plate (entrainment) or by liquid backing up in the downcomers. The lower limit of the vapor flow is set by the condition of weeping, which occurs when the vapor flow is insufficient to maintain the level of liquid on the plate (liquid flows through the holes in the plate). The lower limit of the liquid flow is set by coning. Coning occurs when the vapor flow pushes the liquid back from the holes, jets upwards, with poor liquid contact. The upper limit of the liquid rate is set by the level of the back-up of the liquid in the downcomer.

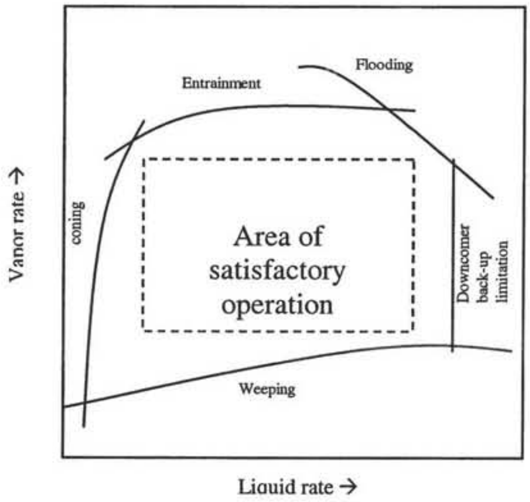

Figure 8-1: Sieve plate performance diagram

The design of a column is a trial-and-error approach and the procedure is described below.

Procedure:

1. Collect or estimate system properties: liquid and vapor flow rates, density of vapor and liquid, surface tension of vapor and liquid, etc.
2. Calculate maximum and minimum vapor and liquid flow rates
3. Estimate tray spacing t_s
4. Estimate column diameter D_c
5. Select liquid flow arrangement
6. Choose provisional plate design: downcomer area, active area, hole area, hole size, weir height
7. Check weeping, if not OK, return to step 6
8. Check plate pressure drop, if too high return to step 6
9. Check downcomer back-up, if too high return to step 3 or 6
10. Recalculate percentage of flooding based on chosen column diameter
11. Check entrainment, if too high return to step 4
12. Optimize design by repeating steps 3 to 11 to find the smallest column diameter and acceptable plate spacing (this will be the lowest cost)

A detailed description of the procedure, together with examples, is given in Appendix 12: Column sizing calculations.

Choices for columns C01, C02 and C03

The tray spacing and column diameter has been calculated as described in the above procedure.

Construction Materials

In the hydroisomerization process there are no exceptional or aggressive chemicals present or extreme temperatures, so the choice of material is the most common and cheapest material: stainless steel for the plates and carbon steel for the column.

Flow arrangement

The selection of the flow arrangement (single pass, double pass) is made with Fig. 11.28 of [24]. Single pass for column C01 and double pass for columns C02 and C03.

Plates

Sieve plates are chosen for all columns, since it is the simplest and cheapest type of plate and there is no special need for other more expensive plate types. The vapor flow rate should not be too low, so no liquid can "weep" through the holes. The hole diameter D_h is set at 5 mm, the weir height h_w at 50 mm (typical values) and the calculations proof that these design specifications are possible. The weir length l_w automatically follows from the selection of the column area, downcomer area and the number of liquid passes of the plates. For all columns the downcomer area A_d is set at 10% of the column area A_c. The calculations prove that with these design values the column is operated within satisfactorily vapor and liquid flow ranges. The most important results are shown below and a calculation example can be found in the Appendices.

Table 8-1: Summary of most important results for C01, C02 and C03

Equipment unit	N (real number of stages) -	D_c (column diameter) m	H_c (column height) m	t_s (tray spacing) m	liquid flow arrangement -
C01	48	3.57	21.2	0.45	single pass
C02	34	5.34	35.2	1.10	double pass
C03	35	5.05	34.0	1.00	double pass

8.2.2 Reactors

This paragraph elaborates more on the background of the reactor specifications, as they can be found in Table 8-2. The complete reactor summary as well as a reactor equipment specification sheet can be found in Appendix 16 and Appendix 17.

Table 8-2: Reactor specifications.

	Reactor 1	Reactor 2
Reactor type	Fixed bed Adiabatic (intercooled)	Fixed bed Adiabatic
Temperature K]	473	573
Pressure $_{in}$ [bar]	9.5	10
Pressure drop [bar]	0.84	0.35
Pressure drop [bar/m]	0.06	0.025
Length [m]	14	14
Diameter [m]	3.7	4.2
Catalyst	Pt/Hβ (0.5 w-% Pt)	Ni/ASA (5 w-% Ni)
Dp [m]	0.003 (sphere)	0.001 (sphere)

Reactor type

Because of their large scale and ease of design and operability, both isomerization reactors, used in the process, are fixed bed reactors. The short residence time distribution of these reactors favors a high selectivity. These reactors can be operated in single-phase or two-phase (trickle flow) mode. Single-phase operation generally is easier however reactor volumes will be larger. In this case very high pressures are required to establish trickle flow. This is not economically feasible and therefore both reactors will be operated in gas phase.

Both reactors will be operated (partly) adiabatic. The kinetics of isomerization and cracking for catalyst I predict a large product loss when the first reactor would be operated fully adiabatic. Therefore this reactor is divided into three zones with intermediate cooling facilities. For catalyst II the product loss is much less pronounced, and this reactor can be operated adiabatic, without any cooling.

Kinetics

The kinetics of isomerization reactions has been described in many scientific papers. The exact mechanism has been under debate. Both ionic mechanisms and the protonated cyclopropane (PCP) route have been mentioned. The PCP route was chosen to be the most probable mechanism. According to this mechanism, 13 reactions involving C7 isomers are possible (see Appendix 23, Appendix 13).

Kinetic data for the chosen catalysts is scarce. The kinetic parameters were obtained by evaluating the results from two papers; Chao et al. [29] for catalyst I, and Emett [30] for catalyst II. Also cracking reactions were taken into account. A detailed description of the procedure is given in Appendix 13.

Pressure drop

Pressure drops through a granular bed can be estimated by means of the Ergun equation:

$$\frac{\Delta P}{L} = A\frac{\varepsilon_P^2}{(1-\varepsilon_P)^3}\frac{\mu \cdot v}{d_P^2} + B\frac{\varepsilon_P}{(1-\varepsilon_P)^3}\frac{\rho \cdot v^2}{d_P} \quad (8.1)$$

with A = 150 and B = 1.75

Reactor sizing

For each catalyst bed the plate thickness is determined, following [24]

The required plate thickness is dependent on the mass of the catalyst that lies on the plate, but also the temperature has an effect. The strength of the material of the plate is expressed in a tensile strength, f, which is dependent on the temperature. This factor is obtained from table 13.2 in [24]. The formula used is:

$$t = C \cdot D^2 \sqrt{\frac{4Mg}{\pi f}} \quad (8.2)$$

For reactor 1 the catalyst mass is distributed over 3 separate beds. The apparent bulk density of the catalyst was assumed to 1000 kg/m^3. The results for the calculation of the plate thickness are presented in Table 8-3.

Table 8-3: Results for the calculation of the plate thickness of both reactors

Parameter		Reactor 1	Reactor 2
T	[K]	473	573
D	[m]	3.7	4.2
Mass catalyst	[kg]	50177	193962
P	[N/m^2]	45803	137410
C		0.43	0.43
f	[N/mm^2]	240	235
t	[mm]	22	44

The required plates are quite thick. In practice support beams will be used. This reduces the effective plate diameter and required thickness.

Also the wall thickness of both reactors is determined. The wall thickness depends on the pressure, the design pressure and the effective diameter, and can be calculated by:

$$e = \frac{p \cdot D}{2f - p} \tag{8.3}$$

For safety a corrosion factor of 2 mm is take into account. Table 8-4 shows the wall thickness for both reactors.

Table 8-4: Wall thickness of both reactors

Parameter		R01	R02
P	[bar]	9.5	10
D	[m]	3.7	4.2
f	[N/mm^2]	240	240
wall thickness	[mm]	7.3	8.8
Corrosion safety factor	[mm]	2	2
Corrected wall thickness	[mm]	10	11

8.2.3 Membranes

Countercurrent Membrane Pervaporation Model

The difference between pervaporation and gas permeation is the driving force for the mass transfer across the membrane. In gas permeation the driving force is the difference in partial pressure of a component on both sides of the membrane. In pervaporation, the driving force is the difference in partial pressure on the gas side and the vapor pressure on the liquid side of the membrane. The advantage of pervaporation over gas permeation is that higher fluxes can be established when the component that needs to be removed from the liquid stream has a relatively high activity, i.e. even at low concentrations it has a strong tendency to evaporate.

The flux in pervaporation can be calculated using the driving force and the permeance value for this specific membrane and this specific component. By using this model it assumed that the individual components do not influence each other's fluxes.

$$J_i = P_i \left(x_i \gamma_i p_i^{sat} - y_i p \right) \qquad (8.4)$$

The mass balances can be specified using the countercurrent plug-flow model (Figure 8-2). Both the composition and the total flow of both streams change and have to be integrated over the length of the membrane.

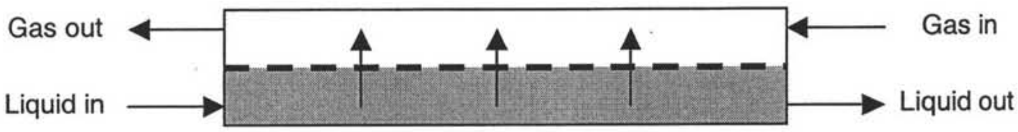

Figure 8-2: Schematic view of countercurrent membrane unit

Component balance for the liquid stream:

$$\frac{d\left(F_L x_i\right)}{dz} = P_i \left(x_i \gamma_i p_i^{sat} - y_i p \right) a_M \qquad (8.5)$$

Component balance for the gas stream:

$$\frac{d\left(F_G y_i\right)}{dz} = P_i \left(x_i \gamma_i p_i^{sat} - y_i p \right) a_M \qquad (8.6)$$

And the total mass balance:

$$\frac{dF_L}{dz} = \frac{dF_G}{dz} = \sum_i P_i \left(x_i \gamma_i p_i^{sat} - y_i p \right) a_M \qquad (8.7)$$

Evaluation of these equations yields the required membrane area (a_M). To evaluate these equations permeance data for the components is required. The data shown in Table 8-5 were estimated using the experimental work of Flanders [4]. For the boundary conditions at the inlet the process streams as calculated by ASPEN were used. The following boundary condition was used for the outlet: The recovery of the slowest permeating species should be >98%. The required membrane area is 200,000 m^2 for the separation of the isomers based on the membrane used by Flanders, which was 100 μm thick. Assuming the permeability is 10 times faster, because a membrane thickness of 10 μm is used in the design instead of 100 μm, the required membrane area is reduced to 20,000 m^2.

Table 8-5: Permeance values and vapor pressure for membrane M01

Permeating component	Vapor pressure at 458 K (bara)	Permeance at 458 K (mol/m^2·s·Pa)
n-C7		10^{-7}
2-MHx		10^{-8}
3-MHx		10^{-8}
3-EP		10^{-8}
2,3-DMP	8.01	10^{-9}
2,4-DMP	9.78	10^{-9}

The concentration profiles along the membrane tube that were calculated using this model are shown here. Only the slowest permeating species were included (2,3-dimethylpentane and 2,4-dimethylpentane):

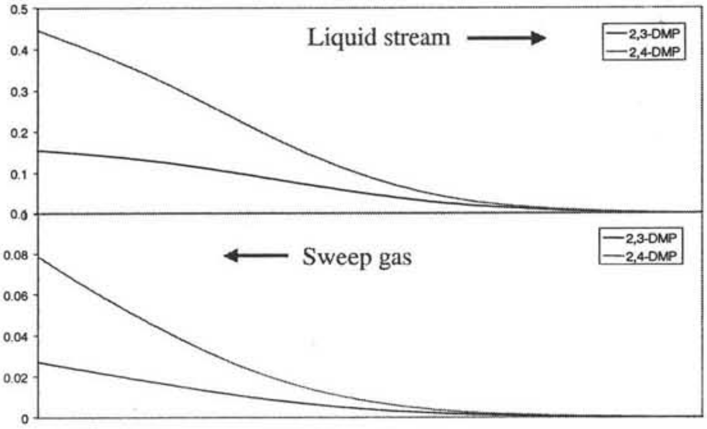

Figure 8-3: Calculated concentration profiles for shell and tube membrane

Next, the dimensions of the membrane unit need to be calculated. Different geometries can be used to apply membrane technology in industrial practice. The most straightforward solution is the shell & tube configuration (Figure 8-4). It is similar to a countercurrent heat exchanger but here mass is exchanged. One of the disadvantages is the large internal volume of the unit (low membrane surface to unit volume ratio). Recently more advanced structures have been developed to use in large scale membrane technology. Monoliths are rigid structures with a very high surface to volume ratio. They consist of a large number of parallel square channels with sizes ranging from 10 to 100 cells per square inch (CPSI). Although in theory these structures can be applied in countercurrent mode (Figure 8-5) it will be practically impossible to connect all individual channels to the corresponding process streams.

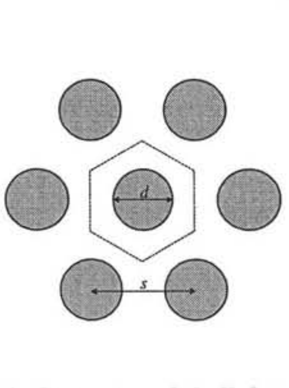

Figure 8-4: Geometry of shell & tube membrane unit (top view)

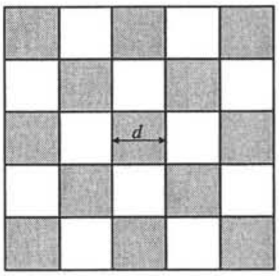

Figure 8-5: Geometry of countercurrent monolith (top view)

A feasible solution is the cross-flow monolith (Figure 8-6). In this structure cross flow can be established because each layer of channels is rotated by 90°. By interconnecting multiple units one can approach countercurrent operation.

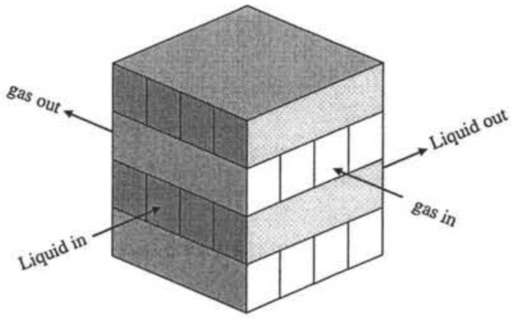

Figure 8-6: Geometry of cross-flow monolith

The dimensions of the shell & tube configuration are calculated as follows (liquid flow inside the tubes):

$$n = \frac{a_M}{\pi d L} \qquad a_L = \frac{\pi}{4} d^2 n \qquad a_G = \frac{\sqrt{3}}{2} s^2 - \frac{\pi}{4} d^2 n \qquad V = \left(a_L + a_G\right) L$$

For both monolith configurations the equations are:

$$n = \frac{a_M}{\beta d L} \qquad a_L = a_G = \frac{1}{2} d^2 n \qquad V = \left(a_L + a_G\right) L$$

Of course, the smaller the tube or channel diameter, the higher the surface to volume ratio will be. This results in a very compact membrane unit design. However, by narrowing the tubes, gas and liquid velocities will increase and so will the pressure drop. This is an important factor for designing membrane units. The liquid velocity and residence time are calculated as follows:

$$u_L = \frac{F_L M}{\rho a_L} \qquad \tau_L = \frac{L}{u_L}$$

And for the gas velocity and residence time:

$$u_G = \frac{F_G R T}{p a_G} \qquad \tau_G = \frac{L}{u_G}$$

Table 8-6: Unit dimensions for two membrane unit options

	Shell & Tube system	Cross-flow monolith
Membrane area	20,000 m^2	20,000 m^2
Channel size	25 mm (tube I.D.)	2.5 mm (100 CPSI)
No. of units	4	1
No. of channels per unit	6366 tubes	$2 \cdot 10^6$ channels
Unit volume	62 m^3	50 m^3
Unit dimensions (LxD or LxWxH)	10x2.8 m	4x4x3.1 m
Liquid velocity	0.7 mm/s	1.5 mm/s
Gas velocity	1.0 m/s	2.2 m/s
Reynolds number (gas)	7500	1650

In this case the limiting factors are not the fluid velocities but the minimal dimensions of current membrane units. For industrial tubes this is around 1 inch tube diameter and for monoliths about 2.5 mm channel size. The results of the calculations are shown in Table 8-6.

For the shell & tube option 4 units with a length of 10 meters are required, each containing 6400 tubes of 1 inch diameter. This option is feasible, but expensive and it will take a lot of space. For the cross-flow monolith option a total volume of 50 m^3 of monolith units with 2.5 mm channels is required. In this case the liquid velocity is 1.5 mm/sec and the gas velocity is 2.2 m/sec. The Reynolds number on the gas side is about 1650, indicating a low pressure drop. This option was chosen for the design.

Hydrogen separation membrane
The data for the hydrogen separation membrane is taken from de [21]. They used a gas separation instead of the forgoing pervaporation model. The designed hydrogen separation membrane is designed as a gas separation, because this is preferable since the feed stream is a vapour stream. The design of the membrane is comparable with the first membrane. The used membrane is an amorphous silica membrane, which is calcined at 400°C. The measured flow through the membrane is F_{H2}= 16.3 m^3STP/m^2.h.bar at a temperature of 473 K. The membrane thickness is only 30 nm, which is possible when sol-gel technology is used.

The pressure difference is dependent on the economics, a high pressure difference means more compressor duty, and is therefore not desirable. But also a low pressure difference is not preferred, because the membrane area increases.
In Table 8-7 the membrane area dependency of the pressure drop is given.

Table 8-7: Membrane surface area dependency of the pressure difference

ΔP bar	A m^2
1	10942
2	5471
3	3647
4	2735
5	2188
6	1824

A pressure drop of 3 bar is chosen because a higher pressure difference would be too expensive, while the membrane is still economic feasible at ΔP = 3bar.
In Table 8-8 the stream specifications are given.

Table 8-8: Stream specifications

F_{feed}	10.6	m3/sec
T	506	K
p	8.66E+05	Pa
ρ	3.1	kg/m3
η	1.44E-05	Pa s

The canal width is taken as small as possible, since a high surface to volume ratio can be achieved. The Reynolds number is maximal 2000, to ensure laminar flow and a low pressure drop. With the data in Table 8-8 the membrane is designed. The results of the membrane dimensions are given in Table 8-9.

Table 8-9. membrane design

D_{canal}	0.002	m
n_{canal}	607881	-
$V_{membrane}$	7.29	m^3
u_g	4.36	m/s
τ_g	0.69	s
Re	1878	-

8.2.4 Pump and compressors

Pumps

An initial pump selection is generally made on the basis of the capacity (flow rate in m^3/h) and the pressure generated. Different charts from literature can be used to determine the type of pump required for a particular head and flow rate. For pumping process fluids, centrifugal pumps will normally be the first choice. [24]

The normal operating range of centrifugal pumps varies from 0.25 – 1000 m^3/s capacity and 10-50 m of water head for single stage pumps to 0.25 – 100 m^3/s capacity and a head of 300 m of water for multistage pumps. [23], [24]. Typical properties of centrifugal pumps are given in Table 8-10.

Table 8-10: Properties of different types of centrifugal pumps [23]

Centrifugal	Max. press. [bara]	Temp. range [K]	Max. diff. press. [bar]	Max. capacity [m^3/s]	Viscosity range [Pa.s]	Efficiency range [%]
Axial	350	33 to 773	2	5	-	50-85 *
Radial	350	33 to 773	20	10	< 0.2	50-85 *
Regenerative	50	243 to 523	35	1.0	< 0.1	20-40 *

* Independent of viscosity up to 0.05 Pa.s

The required pump capacity is determined by the fluid flow. The head can be calculated with the following equation:

$$H = \frac{p_d - p_s}{\rho \cdot g} \qquad (8.8)$$

Where H is the head (m), p_d is the discharge pressure (Pa), p_s is the suction pressure (Pa), ρ is the fluid density (kg/m^3) and g is the gravitational acceleration (m/s^2). [23]

In case a pump is used to transport a fluid over a difference in height the head can be roughly estimated by replacing the term p_d-p_s in equation (8.8) by the static pressure:

$$\Delta P_{stat} = \rho \cdot g \cdot (z_2 - z_1) \qquad (8.9)$$

where z_2-z_1 is the difference in height (m). [23]
An overview of the fluid flows and head for the used pumps can be found in Table 8-11.

Table 8-11: Pump fluid flow and head

Pump	Name	ρ [kg/m³]	Q_p [m³/s]	ΔP [bar]	H [m]	H [m water]
P-01	Reflux C-01	553	0.032	1.39	25.7	14.2
P-02	Reflux C-02	571	0.176	2.22	39.7	22.7
P-03	Bottoms C-02	549	0.058	1.70	31.5	17.3
P-04	Reflux C-03	480	0.162	1.81	38.5	18.6
P-05	Distillate C-03	564	0.024	9.00	162.8	91.7
P-06	Bottoms C-03	555	0.033	8.46	155.5	86.2

The shaft power for pumping an incompressible fluid is given by equation (8.10).

$$Power = \frac{\Delta P Q_P}{\eta_P} \times 100 \qquad (8.10)$$

Where ΔP is the pressure differential across the pump (in N/m^2), Q_p the flow rate (in m^3/s) and η_p the pump efficiency (in %).[24]

Table 8-12 shows a summary of the types and power of the pumps used in the process. A complete pump summary, as well as the pump equipment sheets can be found in Appendix 16 and Appendix 17.

Table 8-12: Pump power and efficiency

Pump	Name	Type	Theoretical power [kW]	η_p [%]	Shaft power [kW]
P01	Reflux C01	Axial Single stage	4	0.72	6
P02	Reflux C02	Radial Single stage	39	0.75	52
P03	Bottoms C02	Axial Single stage	10	0.75	13
P04	Reflux C03	Axial Single stage	29	0.75	39
P05	Distillate C03	Radial Multistage	22	0.68	32
P06	Bottoms C03	Radial Multistage	28	0.72	39

To assure continuous service in total security, pumps are generally provided with an installed spare [22].

Compressors

The selection of compressors is based on flow-rate, the differential pressure required and the operating pressure. Three types of compressors are basically used: reciprocating compressors (high pressures, relatively low flow-rates), centrifugal compressors (high flow-rates and high differential pressures, by staging) and axial flow compressors (high flow-rates and moderate differential pressures). From a diagram by Dimoplon [24] it is estimated that all the compressors in this design have to be centrifugal compressors.

Gas compression causes the gas to heat up and so intermediate cooling is required, usually outside the compressor. Cooling is required because temperatures compatible with compressor technology must be maintained at approximately 493 K [22].
In this design compressor K03 reaches a temperature of 585 K, so intermediate cooling must be applied. A complete compressor summary as well as the compressor equipment sheets can be found in Appendix 16 and Appendix 17.

8.2.5 Heat exchangers

The heat exchangers are sized as described in Coulson & Richardson's Chemical Engineering Volume 6, further mentioned as [24].

The general equation for heat transfer across a surface is:

$$Q = U \bullet A \bullet \Delta T_m \qquad (8.11)$$

where: U = overall heat transfer coefficient [W/m^2 K]
A = heat transfer area [m^2]
ΔT_m = mean temperature difference [K]

An estimate for the overall heat transfer coefficient U is taken from [24]. The mean temperature difference ΔT_m is calculated with:

$$\Delta T_m = F_t \bullet \Delta T_{lm} \qquad (8.12)$$

where: F_t = temperature correction factor, (Fig. 12.19-12.22,[24]) [-]
ΔT_{lm} = logarithmic mean temperature difference [K]

To obtain F_t one has to calculate the dimensionless temperature ratios R and S:

$$R = \frac{T_1 - T_2}{t_2 - t_1} \qquad (8.13)$$

$$S = \frac{t_2 - t_1}{T_1 - t_1} \qquad (8.14)$$

where: T_1 = inlet shell-side fluid temperature [K]
T_2 = outlet shell-side fluid temperature [K]
t_1 = inlet tube-side fluid temperature [K]
t_2 = outlet tube-side fluid temperature [K]

The logarithmic mean temperature difference ΔT_{lm} [K] is:

$$\Delta T_{lm} = \frac{(T1\text{-}t2)\text{-}(T2\text{-}t1)}{\ln \frac{T1\text{-}t2}{T2\text{-}t1}} \qquad (8.15)$$

When no phase change occurs, the heat duty Q [kW] of a stream is:

$$Q = \Phi_m \bullet Cp \bullet (T_{out} - T_{in}) \qquad (8.16)$$

where:			
	Φ_m =	mass flow of stream to be heated or cooled	[kg/s]
	Cp =	specific heat	[kJ/kg K]
	T_{out} =	outlet stream temperature	[K]
	T_{in} =	inlet stream temperature	[K]

If a phase change occurs, the heat duty of a stream is:

$$Q = \Phi_m \bullet \left[Cp \bullet (T_{out} - T_{in}) + \Delta H_{vap} \right] \qquad (8.17)$$

where: ΔH_{vap} = heat of vaporization (or condensation) [kJ/kg]

The overall heat transfer coefficient U is estimated with [24]. With, Q, U and ΔT_m known, the necessary heat transfer area is calculated.

Choices made for heat exchanger E10

For heat exchangers the designer can choose several types of heat exchangers, which are listed in Table 8-13.

Table 8-13: Heat exchanger types.

Type	Reasons for use
Shell & tube heat exchanger	Most commonly used in the chemical industry, because: • Large surface area in small volume • Good shape for pressure operation • Well-established fabrication techniques • Can be constructed from wide range of materials • Easily cleaned • Well-established design procedures
Gasketed plate heat exchanger	Extensively used in food and beverage industry. Not good shape to resist pressure. Limited to about 30 bar and 250 °C
Welded plate heat exchanger	Up to 80 bar and 500 °C
Plate-fin heat exchanger	Large surface area. Up to 60 bar and 150 °C. Unit cannot be mechanically cleaned, so use restricted to clean streams
Spiral heat exchanger	In general compact: large area, small volume. Up to 20 bar and 400 °C. Low pressure drop (compared to shell and tube)
Direct contact heat exchanger	No general design method exists
Double pipe heat exchanger	Simplest and cheapest heat exchanger. Used when small heat exchanger area required
Air cooled	Used when cooling water is short in supply. Can be economically more attractive above specific temperature (ca. 100-120 °C)
Fired heaters	Used when high temperatures and flow rates are required. Capacity ranges from 3 to 100 MW

Only a description of the design of heat exchanger E10 is described below. All other exchangers are designed in the same way. The only major difference between the design calculations of all heat exchangers is the estimation of the shell-side and tube-side coefficient and temperatures. If there is a phase change and there are two phases present, the correlations used are different than if there is no phase change (and only one phase present). If there is only one temperature on either the shell or tube side (e.g. condensation or vaporization), then the logarithmic temperature difference will be simplified.

Heat exchanger E10 (heating)

Type

Shell & tube heat exchanger is chosen for the reasons listed in Table 8-13 and because shell & tube heat exchangers are the most commonly used heat exchangers in an oil refinery. E10 will operate at tube-side pressures of 40 bar (HP steam) and shell-side pressure of 10 bar. The logarithmic mean temperature difference (LMTD) is 192.5 K. In Table 8-14 the algorithm for choosing the type of shell & tube heat exchangers is demonstrated: a shell & tube, one pass tube, one pass shell (E shell) heat exchangers is chosen for E10. There is no excessive heat transfer area or heat duty required, so there is no need for more complex exchanger equipment than the (simple) E shell. At this stage of the process design it is not necessary to determine whether an internal or external floating head heat exchanger is necessary.

Table 8-14: Algorithm for choosing shell & tube heat exchanger type for exchanger E10.

Type (Shell & Tube)	Reason	Possible yes/no?
fixed tube sheet	temperature difference too high ([24]suggest max difference of 80 K) and shell pressure limited to 8 bar	No
floating head	shell-side pressure usually limited to 20 bar: in our case OK. Shell side and Tube side at different pressure and temperature	Yes
U-tubes	U-tube suitable for high temperature differentials and bundle can be easily removed and shell cleaned. Tubes can't be easily cleaned	No
finned tubes	Used when heat transfer coefficient on outside tube is appreciably lower that on inside tube (e.g heat transfer liquid to gas). Finned exchanger will increase effective surface area: not necessary	No

Orientation

Horizontal orientation is chosen, because:

- No extra pressure (head) to overcome
- Easier and cheaper construction
- Easier servicing

Construction Material

Carbon steel is used as construction material for the heat exchangers, because:

- No extreme pressures and temperature differences occur
- No extreme corrosion precautions necessary
- Relatively cheap

Utility

The C7 stream needs to be heated from 360 K to 458 K. MP steam (10 bar) and HP steam (40 bar) have a condensing temperature of 453 K and 523 K respectively: select 40 bar HP steam.

Fluid allocation: Shell side vs Tube side

The method for allocating the streams is demonstrated in Table 8-15.

Table 8-15: Allocation of streams for E10.

Factor	**Allocation**	**This case**	**conclusion**
Corrosion	Most corrosive fluid on tube side, because this will reduce costs of expensive alloy	na	na
Fouling	Fluid with greatest tendency to foul on tube side, which will give better control over fluid velocity	Fouling almost equal assumed	na
Fluid temperatures	At moderate temperatures, hotter fluid on tube side	Steam hotter	Tube: Steam Shell: C7
Operating pressures	Higher pressure stream on tube side	Steam higher pressure	Tube: Steam Shell: C7
Pressure drop	Flow with lowest allowable pressure drop on tube side	na	
Viscosity	More viscous material to shell side, in general, will give higher heat transfer coefficient	Steam is less viscous	Tube: steam Shell: C7
Stream flow rates	Lowest flow rate on shell side will give most economical design	Steam has lowest flow rate	Tube: C7 Shell: steam
General Conclusion:			**Tube side (hot): steam** **Shell side (cold): C7**

Overall heat transfer coefficient

The overall heat transfer coefficient is determined with the help of Fig. 12.1 and Table 12.1 of [24]. For heat exchanger E10 the overall heat transfer coefficient U is estimated at 850 W/m^{2}K.

Table 8-16: Summary of results for heat exchangers.

Exchangers	Service	Heat transfer coefficient (estimate) [W/m^2 K]	Utility
E01, E03, E05	Condensor	600	Cooling water
E02, E04, E06	Reboiler	950	LP steam
E07	vaporizer	950	HP steam
E10	Heat exchanger	850	HP steam
E11	Heat exchanger	250	Cooling water

8.2.6 Furnace

Assumptions:

- The heat transfer to the tubes of the furnace walls is dominanated by radiation and for this design, it is assumed to be only radiation
- For most applications the heat flux to the tubes q_r is between 20 and 40 kW/m^2. For a rough estimate of the tube area needed, a value of 30 kW/m^2 is used for q_r
- Tube diameters are normally between 75 and 150 mm and for this design a value of 150 mm is used
- Typical tube velocities are between 1 and 2 m/s and for this design a value of 1.5 m/s is used
- Modern fired heaters operate at thermal efficiencies of 80 to 90 % and for this design a value of 85 % is used
- The heat of combustion $\Delta H_{combustion}$ is assumed to be the same as the average heat of combustion of the lights in the process (stream nr. 18 in the stream summary, Appendix 2). The value is 45,200 kJ/kg.

The preliminary design for the furnace is done as described in [24].

Calculation of the total area of the tubes:

$$\Delta H_{gas} = A_{tubes} \bullet q_r \tag{8.1}$$

where: ΔH_{gas} = enthalpy difference in gas to be heated, heat duty required [kW]
A_{tubes} = total area of tubes [m^2]
q_r = radiant heat flux [kW/m^2]

The total number of tubes can be calculated with:

$$\Phi_{v,gas} = N_t \bullet A_{cross,tube} \bullet v_{gas} \tag{8.2}$$

where: $\Phi_{v,gas}$ = volumetric flow rate of gas to be heated [m^3/s]
N_t = total number of tubes [-]
$A_{cross,\ tube}$ = cross-sectional area of one tube [m^2]
v_{gas} = velocity of gas to be heated [m/s]

The amount of fuel necessary can be calculated with:

$$\Delta H_{gas} = 0.85 \bullet \Phi_{m,fuel} \bullet \Delta H_{combustion} \tag{8.3}$$

where: $\Delta H_{combustion}$ = heat of combustion [kJ/kg]
$\Phi_{m,fuel}$ = mass flow rate of fuel necessary [kg/s]

The calculations are demonstrated in Appendix 15. The furnace needs to have 91 tubes with a total area of 208.1 m^2. The amount of fuel necessary is 14.0 t/d.

9. WASTE MANAGEMENT

9.1 DURING CONTINUOUS OPERATION

The different waste streams and their destinations are summarized in Table 9-1. The hydrogen purge waste stream can be reused as fuel gas in the furnace.

Table 9-1: Waste stream summary

Waste stream	Contents	Destination
H_2 purge	Hydrogen, trace impurities	Fuel gas
Exhaust gas furnace	CO_2, H_2O, impurities	Stack

9.2 DURING START-UP

At process start-up the distillation columns are started one at a time and then operated in total reflux mode until each of them is in equilibrium. During this period the feed flow is bypassed directly to the reformer, and there are no waste streams.

At the same moment, both catalyst beds in the reactors need to be activated (reduced). This is accomplished by feeding a hot hydrogen stream (possibly diluted with nitrogen) at atmospheric pressure through the reactors. During the reduction process, water vapor is formed which leaves the reactor in the outlet stream. The outlet stream contains hydrogen, water and nitrogen, and can be fed to the furnace fuel stream.

When the catalyst activation is complete, the hydrogen recycle loop can be started. During this process some of the recycle stream should be purged, as trace impurities might accumulate in the loop. When the recycle flow and temperature is stable, the feed flow to the reaction can be started. After a stabilization period, the process will reach steady state continuous operation.

9.3 DURING SHUTDOWN

When the process needs to be shut down, for example to replace the catalyst, the feed intake is stopped and the whole system is purged by opening the purge valves and relieving the pressure. The reactors are flushed with hydrogen and nitrogen to remove all reactive components. The offgas stream can be fed to the furnace.

The catalyst is pyrophoric. This means that it can burn instantaneously upon exposure to air. Thus, the removal of the catalyst is a dangerous routine, usually carried out by specialists from the catalyst manufacturing company.

The spent catalyst contains Si, Al, Ni and Pt oxides and is usually reclaimed by the catalyst manufacturer for recycling.

Summarizing, during start-up and shutdown no additional waste streams are created, only the spent catalyst needs to be disposed of.

10. PROCESS SAFETY

A DOW Fire & Explosion Index analysis was performed for all process units with a large hold-up, followed by a HAZOP study for the most dangerous process unit.

10.1 DOW FIRE & EXPLOSION INDEX

The complete procedure for estimating the most important aspects of the F&EI, was followed as described in [25]. A summary of the results is presented in Table 10-1. A more detailed description for the most dangerous process unit, the furnace, is given as an example. The F&EI sheet can be found in Appendix 18. It is assumed that the operation condition for all examined units is normal.

Table 10-1: Process units, Material Factors, F&E Index, Area of exposure and damage factors.

Process Unit	MF	F&EI	Area of exposure [m^2]	Damage factor
C01 Tailing Column	21	60	740	0.56
C02 Topping Column	21	66	897	0.60
C03 Reactant Separation Column	21	64	831	0.58
F01 Feed R02 heating furnace	21	93	1800	0.70
R01 Reactor 1	21	78	1246	0.65
R02 Reactor 2	21	78	1259	0.65
M01 Product Separation Membrane	21	65	873	0.60
M02 Hydrogen Separation Membrane	21	64	852	0.59

10.1.1 Determination process units and material factor

First a selection was made on the plot plan of the Pertinent Process Units that are considered of key importance to the process and that would have the greatest impact on the magnitude of a potential fire or explosion. This resulted in eight process units, namely all distillation columns, the reactors, both membranes and the furnace.

Next a determination was made of the Material Factor (MF) for each process unit. The MF is obtained from the NFPA ratings N_F and N_R. If the temperature of the material on which the MF is based is over 60 °C, an adjustment is required. [25]
All process compounds and their MF can be found in Appendix 18.
As it seemed that the furnace operates at a temperature that crosses the value of 60 °C, the MFs become 21 for all the materials heated by the furnace. Therefore the overall MF for the furnace has a value of 21, and components in the relevant streams have to be taken into account for the determination of the F&EI.

10.1.2 Determination general process hazards (F1)

The general process hazards are very basic hazards and can be applied to most process situations. In the furnace no reactions take place, no material handling and transfer is needed. It is assumed that the location of the furnace is outside and the access to the unit is sufficient. Drainage and spill control is not present, so therefore a penalty of 0.5 is applied. The total General Process Hazards Factor (F_1) has a value of 1.5.

10.1.3 Determination special process hazards (F_2)

Special process hazards consist of specific process conditions that could be major causes of fire and explosion accidents.

The highest N_F factor of all compounds present in the furnace is 1, so therefore the penalty for toxicity becomes 0.2. The operation of the furnace is only in the flammable range with a process upset, and the penalty for this is 0.3. The penalty for an operating pressure of 1 bar is calculated by means of the formula given in page 22 of [25] and has a value of 0.37. Corrosion and erosion will occur slightly, so this penalty factor is set to the minimum of 0.1. The penalty for the use of fired equipment is set to the maximum of 1.0. The total Special Process Factor (F_2) has a value of 2.97. The hold-up of the furnace is very low, so the penalty for the quantity of flammable material is not determined.

10.1.4 Total F&E Index

The Process Units Factor (F_3) is calculated by multiplying the values of F_1 and F_2, and has for the furnace a value of 5.20. This is within the normal range of 1-8. The total value of the F&E index is calculated by multiplying the MF with F_3.

The furnace has a F&EI of 93, which means a moderate degree of hazard. The value for the furnace F&EI does not exceed the value of 128, so no further risk review has to be done.

10.1.5 Additional risk information

The radius of exposure is calculated by multiplying the F&EI with 0.84. For the furnace this radius is 24 m, therefore the area of exposure becomes 1800 m^2.

The damage factor can be estimated with the help of figure 8 of [25] and has a value of 0.7. See Table 10-1.

10.2 HAZOP

Although the most dangerous process unit is the heating furnace, a HAZOP study was done for the second most dangerous process unit, reactor 2. A furnace is very common, and therefore it was more educational to do a HAZOP study for a less common process unit.

Table 10-2 shows the results of the performed HAZOP

Table 10-2: HAZOP study for Reactor 2.

Guide Word	Deviation	Causes	Consequences	Actions
NO NOT	No Inlet Flow	(1) Compressor failure (2) Line rupture (3) Line blockage	(1) Reactor runs empty (2) Hydrogen/hydrocarbon vapor discharged into atmosphere, possible vapor cloud explosion (3) Pressure buildup in compressor	(1) Regular maintenance of compressor (2) Regular inspection and maintenance of piping (3) Regular inspection and maintenance of piping
	No Outlet Flow	(4) Reactor rupture (5) Reactor blockage	(4) Hydrogen/hydrocarbon vapor discharged into atmosphere, possible vapor cloud explosion (5) Pressure buildup in reactor	(4) Regular inspection and maintenance of reactor (5) As in (4), install pressure safety
	No Hydrogen in Inlet Flow	(6) Ratio flow control failure	(6) Severe product cracking, Coking of catalyst	(6) Regular testing of control loop
	No Hydrocarbon in Inlet Flow	(7) Membrane (M01) failure	(7) No reaction, no product	(7) Regular maintenance of membrane unit
LESS	Less Inlet Flow	(8) Compressor malfunction (9) Line leakage (10) Line plugging	(8) Lower conversion, higher purge flow (9) Hydrogen/hydrocarbon vapor discharged into atmosphere, possible vapor cloud explosion (10) Pressure buildup in compressor	(8) Regular maintenance of compressor (9) Regular inspection and maintenance of piping (10) Regular inspection and maintenance of piping
	Less Outlet Flow	(11) Reactor leakage (12) Reactor plugging	(11) Hydrogen/hydrocarbon vapor discharged into atmosphere, possible vapor cloud explosion (12) Pressure buildup in reactor	(11) Regular inspection and maintenance of reactor (12) As in (11), install pressure safety
	Less Hydrogen in Inlet Flow	(13) Ratio flow control failure (14) Membrane (M02) plugging	(13) More product cracking (14) More product cracking	(13) Regular testing of control loop (14) Regular maintenance of membrane unit
	Less Hydrocarbon in Inlet Flow	(15) Membrane (M01) plugging	(15) Less product	(15) Regular maintenance of membrane unit
	Lower Temp	(16) Furnace failure (17) T control failure	(16) Lower conversion, higher purge flow (17) Lower conversion, higher purge flow	(16) Regular maintenance of furnace (17) Regular testing of control loop

	Lower Pressure	(18) Compressor malfunction (19) Outlet pressure control failure (20) Reactor leakage (21) Line leakage	(18) Lower conversion, higher purge flow (19) Lower conversion, higher purge flow (20) Hydrogen/hydrocarbon vapor discharged into atmosphere, possible vapor cloud explosion (21) As in (20)	(18) Regular maintenance of compressor (19) Regular testing of control loop (20) Regular inspection and maintenance of reactor (21) Regular inspection and maintenance of piping
MORE	More Inlet Flow	(22) Feed flow control failure (23) Recycle flow control failure (24) Membrane (M01) failure	(22) Lower product yield (23) Lower product yield, more cracking (24) Lower product yield	(22) Regular testing of control loop (23) Regular testing of control loop (24) Regular maintenance of membrane unit
	More Hydrogen in Inlet Flow	(25) Ratio flow control failure	(25) Lower product yield	(25) Regular testing of control loop
	More Hydrocarbon in Inlet Flow	(26) Membrane (M01) failure	(26) Lower product yield	(26) Regular maintenance of membrane unit
	Higher Temp	(27) Furnace failure (28) T control failure	(27) Lower product yield, more cracking (28) Lower product yield, more cracking	(27) Regular maintenance of furnace (28) Regular testing of control loop
	Higher Pressure	(29) Compressor malfunction (30) Outlet pressure control failure	(29) Lower product yield, more cracking (30) Lower product yield, more cracking	(29) Regular maintenance of compressor (30) Regular testing of control loop
REVERSE	Reverse Flow	(31) Compressor failure (32) Line Rupture	(31) No reaction, no product (32) As (2)	(31) Regular maintenance of compressor (32) As (2)
AS WELL AS	Product isomers in Feed	(33) Membrane (M01) failure	(33) Lower product yield, more cracking	(33) Regular maintenance of membrane unit

11. ECONOMY

11.1 CALCULATION OF COSTS

The economical performance of the plant is based on a 350 days a year operation.
In the next paragraphs the total investment, the operating cost, income and cash-flow are described. The method is based on the method described in [24]

Total investment
The fixed capital is the total cost of the plant ready for start-up and can be estimated with the factorial method of Lang. The fixed capital cost of the project is given as a function of the total purchase equipment cost by the equation

$$C_F = f_L Ce \qquad (11.1)$$

Where C_F is the fixed capital cost, f_L is the Lang factor, which depends on the type of the process and Ce is the total delivered cost of all major equipment items. In Table 11-1 the Lang factors are given.

Working capital is the additional investment needed, over and above the fixed capital, to start the plant, and to operate it to the point when income is earned. The working capital is typical 15 % for petrochemical processes.

Table 11-1. Lang factors

Item	F	Lang factor
Major equipment		
Equipment erection	f_1	0.4
Piping	f_2	0.7
Instrumentation	f_3	0.2
Electrical	f_4	0.1
Buildings, process	f_5	0.15
$f_1+\ldots+f_5$		1.55
Fixed capital		
Design and engineering	f_6	0.3
Contractor's fee	f_7	0.05
Contingency	f_8	0.1
$f_6+f_7+f_8$		0.45

The total physical plant cost can be estimated with

$$PPC = PCE(1+f_1+...+f_5) = 2.55 \cdot PCE \qquad (11.2)$$

The Fixed Capital can now be estimated with:

$$C_F = PPC(1+f_6+f_7+f_8) = 1.45 \cdot PPC = 3.70 \cdot PCE \qquad (11.3)$$

The purchase costs are estimated with DACE, 2000, the method in Douglas and with the method given in [24, table 6.2]
The membrane costs are taken fl 360,- per m^2. Where M01 has a surface area of 20000 and M02 a surface area of 4000 m^2.

Table 11-2. Total equipment cost

Equipment	design name	Price (Mfl)
Distillation columns	C01-C03	3.74
Heat exchangers	E01-E12	3.6
heater feed R02	F01	0.6
Compressors	K01-K03	3.8
Membranes	M01-M02	8.6
Pumps	P01-P06	0.25
First reactor	R01	0.11
Second reactor	R02	0.12
PCE	[Mfl]	20.82

Now the fixed capital cost can be estimated

$$C_F = f_L \cdot Ce = 3.70 \cdot PCE = 77.03\ Mfl$$

Table 11-3. Total investment

Investment		[Mfl]
Fixed Capital	C_F	77.03
Working Capital	$0.15 \cdot C_F$	11.56
Total investment	$1.15 \cdot C_F$	88.59

Operating/production costs

These costs include all expenses that are made on a continuous basis per year. These expenses are divided in costs that are directly related to the operation and in costs that are indirectly related to the operation e.g. taxes, insurance etc.

The direct costs are divided in variable costs, like the costs of the raw material and in fixed costs like labor costs.

In the operation costs also the catalyst is taken into account, since the catalyst needs to be replaced every 2 years. The catalyst costs are assumed as operation costs, since they are not an investment. The platinum is leased, because to buy the platinum is a big investment. It is assumed that the lease percentage is 10 % per year of the cost price of platinum for the whole catalyst bed. The weight of platinum used is 750 kg, which costs 24.53 Mfl.

Table 11-4. Catalyst cost data [9]

	Catalyst 1		Catalyst 2
Platina price/ kg	32700.00	Nickel	12
Platina 0.05 wt%	163.5	Nickel 5 wt %	0.6
Hbeta	70	Silica alumina	15.7
Total price FL/ kg	234		16

The operating costs, the costs of producing the product, can be divided in direct and indirect costs. These costs can be estimated from the flowsheet and the capital cost estimate. In Table 11-5 a summary of the production costs is shown.

Table 11-5. Summary of the production costs

Variable costs	Mfl/a	
Raw materials		117.15
Catalyst	Regenerated every 2 years	7.00
24.525 Mfl Plat. Costs	Platina lease 10%	2.45
Utilities	(electricity + steam + cooling)	43.78
Total variable costs	170.4	
Fixed costs		
Maintenance	5 % of CF	3.852
Operating labor	fl 100000 1) 5 shifts x 4 men = 20	2
Laboratory costs	20% of operating labor	0.4
Supervision	20% of operating labor	0.4
Plant overheads	50 % of operating labor	1
Capital charges	10 % of CF	7.7
rates (taxes)	1 % of CF	0.77
Insurance	1 % of CF	0.77
Royalties	1 % of CF	0.77
total fixed costs		17.66
Total direct costs		188.04
Indirect costs General overheads, R& D costs, Sales expense.		9.4
Total indirect costs		9.4
Annual operating costs		197.44
Operating costs/ kg product	fl / tonne product	2559.07

1) For a continuous process, 5 shifts are needed and 4 persons per shift.

Annual income

The annual income is a summation of all the sells of the products and by-products. In Table 11-6 the prices of the streams and the profit are given.

Table 11-6. Sales of product and byproducts

Stream	Price stream fl/t	Mass flow t/d	Mass flow t/a	Income Mfl/a
Product	1035.07	220.44	77154	79.86
Light	852.05	260.35	91123	77.64
Heavy	315.97	397.62	139167	43.97
Purge	55.13	31.89	11162	0.62
Total		910.30	318500	202.09

The net cash-flow is 202.09- 197.44= 4.65 Mfl/a

11.2 ECONOMIC EVALUATION

Now that the total investment, operating costs and the net cash-flow are determined the process profitability can be evaluated. This is done by the discount cash-flow analysis, were the time value of money is taken into account. From this analysis the rate of return (ROR) and the pay back time (PBT) can be determined.

During the first two years the capital costs are paid to build the plant and there is no income or operating costs. After these two years the net cash-flow is the income where the bills have to be paid of. The discounted cash-flow is calculated by

$$NPW = \sum_{n=1}^{n=t} \frac{NFW}{(1+r)^n} \tag{11.4}$$

Where *NPW* is the net present worth, *NFW* is the net future worth, *r* is the interest rate and *n* is the year of the NFW.
In this case r is 10 % which is suggested by [20].

In table 2 in Appendix 20 it can be seen that the net present worth (cum. discounted cash flow) at 10 % means a great loss. This could already be foreseen, because the maximum allowable investment at an interest rate of 10 % and a project lifetime of 10 years is 31 Mfl (See Appendix 20, table 1), while the current investment is 89 Mfl. In Figure 11-1 the project cash flow is shown.

The discount cash-flow rate of return can be determined to change the interest so that NPW is zero. The DCFRR is determined by trial and error and is - 9,5%. This means the plant has to be sponsored to equal investments

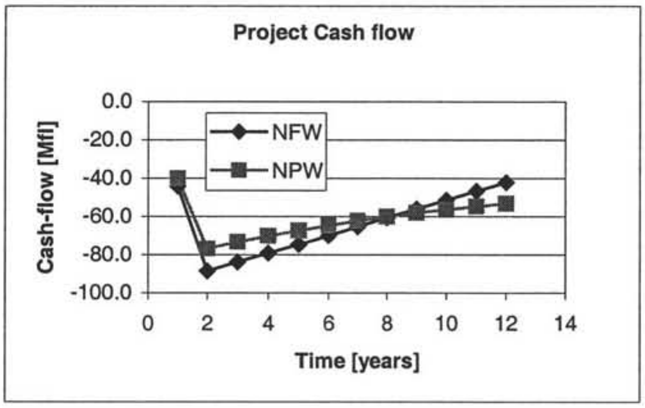

Figure 11-1. Project cash-flow

The rate of return is the ratio of annual profit to investment, which can be calculated with the following formula

$$ROR = \frac{Cumulative\ net\ cashflow\ at\ end\ of\ project}{life\ of\ project \cdot original\ investment} \cdot 100\%$$

$$ROR = \frac{-42.128}{10 \cdot 88.6} \cdot 100\,\% = -4.75\,\%$$

The pay back time is the time required after the start of the project to pay off the initial investment from income.

$$PBT = \frac{Total\ investment}{cash - flow}$$

$$PBT = \frac{88.6}{4.65} = 19\ years$$

11.3 SENSITIVITY ANALYSIS

In this section a check is made upon the influence of product and hydrocarbon feed prices on the process profitability. The influence of price changes is investigated by calculating the NPV of the process using a price that differs a certain percentage from the current price. Also the utility costs and the total investment are varied to investigate the influence on the maximum allowable investment. As soon the maximum allowable investment exceeds the current investment the process is profitable within the process lifetime.

The results are given in Table 11-7. It can be seen that the process can be profitable when the feed price decreases with 10%, or when the product price increases with 6%.

Table 11-7. Sensitivity analysis

Variation	Operational costs	Income	Margin	Max. investment	Calculated investment
%	Mfl/a	Mfl/a	Mfl/a	Mfl/a	Mfl/a
Variation Feed price					
-15	178.99	202.09	23.10	117.3	88.6
-10	185.14	202.09	16.95	86.1	88.6
-5	191.29	202.09	10.80	54.8	88.6
0	197.44	202.09	4.65	23.6	88.6
5	203.59	202.09	-1.50	-7.6	88.6
Variation Product price					
-10	197.44	181.9	-15.54	-79	88.6
-5	197.44	192	-5.44	-27.7	88.6
0	197.44	202.09	4.65	23.6	88.6
5	197.44	212.19	14.75	74.9	88.6
6.4	197.44	215	17.56	89.3	88.6
10	197.44	222.3	24.86	126.2	88.6
Variation investment					
-10	196.8	202.09	5.29	26.9	79.7
-5	197.12	202.09	4.97	25.2	84.2
0	194.44	202.09	7.65	23.6	88.6
5	197.77	202.09	4.32	22	93.0
10	198.09	202.09	4.00	20.3	97.5
Variation utility costs					
-10	192.88	202.09	9.21	46.9	88.6
-5	195.14	202.09	6.95	35.3	88.6
0	197.44	202.09	4.65	23.6	88.6
5	199.74	202.09	2.35	11.9	88.6
10	202.04	202.09	0.05	0.2	88.6

11.4 DISCUSSION

From the foregoing it can be seen that the process is not profitable.

The main problem is the product price, because the current gasoline prices are taken to calculate the price per RON-number. The octane-booster MTBE for example is relative cheap, while it has a high RON. Therefore the prices for current gasoline are too low to produce gasoline with multibranched heptane. Increasing the gasoline price can solve the problem. This can be defended by the argument that the current gasoline is very bad for the environment, while the new product is much better and satisfies the future demands.
From the sensitivity analysis it can be seen that the product price only has to increase 6% to make the process profitable.

In the process itself also savings are possible when for example the reactors could have a smaller volume what would save catalyst, or when a better membrane is available so less surface area would be needed.
Another big investment are the compressors, if less hydrogen can be used it would not only save investment costs but also energy.
However the sensitivity analysis shows that savings on the total investment or utilities is much less profitable than changing the feed or product price.

12. CONCLUSIONS AND RECOMMENDATIONS

12.1 TECHNICAL FEASIBILITY

This conceptual process design shows, that by using the latest membrane separation technology, a heptane hydroisomerization plant can be built. All unit operations are technically realizable and have realistic dimensions.
A total amount of 907 tonne/day, this is 317500 tonne/a, feed is processed from which 220 tonne/day, which is 77000 tonne/a, product is formed. This means a product yield of 4.1 tonne feed per tonne product. The plant is on stream for 350 days a year, so maintenance can be done for 15 days a year, the on-stream factor is therefore 0.96.

The selectivity towards the desired product 2,2,3-TMB is 20%. The conversion of n-heptane in the first reactor is 49% and the conversion of 2,4-DMP in the second reactor is 41%.

12.2 ECONOMIC FEASIBILITY

The economic evaluation indicates a negative cash flow during the 10-year operational life of the plant, given the current prices for feed and products. A product price increase of 6.4 percent is needed to attain a positive cash flow. Another possibility is to reduce the feed price with 10.5 %
The operating costs per tonne product are 2559 fl/tonne product. The investment costs per tonne product produced in 10 years are 114.8 fl/tonne.

12.3 SAFETY AND ENVIRONMENT

It is shown by HAZOP and F&EI studies that all unit operations can be operated without extreme risk potential. Most of the byproduct streams generated by the process can be reused or sold. The remaining waste streams can be disposed in a proper way.

12.4 RECOMMENDATIONS

One of the limitations of this conceptual process design is the relatively large uncertainty in the parameters that were used to simulate the reactors and membranes. The kinetic data for both reactors is based on simple conversion data from one single experiment described in literature.
Because of lack of information on temperature dependence of the kinetics, the reactors are operated at the temperatures given in literature. However a lower temperature would assure less cracking and a higher conversion to isomerisation, which is preferred. It is therefore recommended to investigate the performance of the used catalysts at varying temperatures.
Also the hydrogen to feed ratio could be investigated, since at lower temperature less cracking will occur. This would reduce reactor volume, compressor duty and hydrogen costs.

The permeation data for the membrane are estimated from one experiment describing the permeation of C6 isomers. It is highly recommended to elaborate on these points, to do more kinetic measurements and to measure permeance values for relevant pure components and mixtures. The feed, which is produced in the hydrotreater, is a complex mixture with a wide range of components varying from C5 to C11. The feed is simplified, because the kinetic model is based on conversions of linear C7. All other components are therefore left out the simulation. It is especially recommended to investigate the behavior of cyclic and aromatic compounds.
Attention should be paid to a better estimation than the rough estimation of the product- and feed prices, which are based on current gasoline prices and RON numbers in this report.

LIST OF SYMBOLS

Chapter 3:

RON_i	Research Octane Number of component i
x_i	Molefraction of component i
NFW	Net Future Worth (Mfl/a)
NCF	Net Cash Flow (Mfl/a)
DCF	Discount Cash Flow (Mfl/a)
$DCFROR$	Discount Cash Flow Rate Of Return (%)

Chapter 8.2.2 Reactors

A	Constant
B	Constant
C	Constant
D	Internal reactor diameter (m)
d_p	Particle diameter (m)
e	Wall thickness (m)
f	Design stress for low alloy steel at given T (Pa)
ε_p	Particle porosity (-)
g	Gravitational acceleration (m/s^2)
L	Bed length (m)
M	Catalyst bed mass (kg)
μ	Fluid viscosity (Pa·s)
ΔP	Pressure drop (Pa)
ρ	Fluid density (kg/m^3)
t	Plate thickness (m)

Chapter 8.2.3 Membranes

a_G	Cross sectional area for gas flow (m^2)
a_L	Cross sectional area for liquid flow (m^2)
a_M	Membrane area (m^2)
β	β=2 for countercurrent, β=1 for cross-flow configuration (-)
d	Diameter of membrane tubes or monolith channels (m)
F_G	Molar flow of gas stream (mol/s)
F_L	Molar flow of liquid stream (mol/s)
γ_i	Activity coefficient of component i in liquid stream (-)
J_i	Flux of species i through membrane (mol/m^2s)
L	Total length of membrane unit (m)
M	Average molar mass of liquid stream (mol/kg)
n	Number of membrane tubes or monolith channels (-)
P_i	Permeance of component i (mol/m^2sPa)
p	Pressure in gas stream (Pa)
p_i^{sat}	Vapor pressure of pure component i in liquid stream (Pa)
ρ	Average density of liquid stream (kg/m^3)
R	Gas constant (J/molK)
s	Spacing of membrane tubes (m)
τ_G	Residence time of gas stream in membrane unit (s)
τ_L	Residence time of liquid stream in membrane unit (s)
T	Temperature (K)

u_L	Velocity of liquid stream (m/s)
u_G	Velocity of gas stream (m/s)
V	Total volume of membrane unit (m^3)
x_i	Molefraction of component i in liquid stream (-)
y_i	Molefraction of component i in gas stream (-)
z	Axial space coordinate (-)

Chapter 8.2.4:

H	Pressure head (m)
p_d	Discharge pressure (Pa)
p_s	Suction pressure (Pa)
ρ	Fluid density (kg/m^3)
G	gravitational acceleration (m/s^2)
ΔP_{stat}	Static pressure difference (Pa)
z	Vertical position (m)
Q_p	Flow rate (m^3/s)
η_p	Pump efficiency (%)

Chapter 11:

C_F	Fixed capital cost (Mfl/a)
f_L, f_i	Lang factors
Ce	Total delivered cost of all major equipment items (Mfl/a)
PPC	Total Physical Plant Cost (Mfl/a)
PCE	Physical Cost of Equipment (Mfl/a)
NPW	Net Present Worth (Mfl/a)
NFW	Net Future Worth (Mfl/a)
r	Interest rate (%)
n	Year of the NFW
ROR	Rate Of Return (%)
PBT	Pay-Back Time (years)

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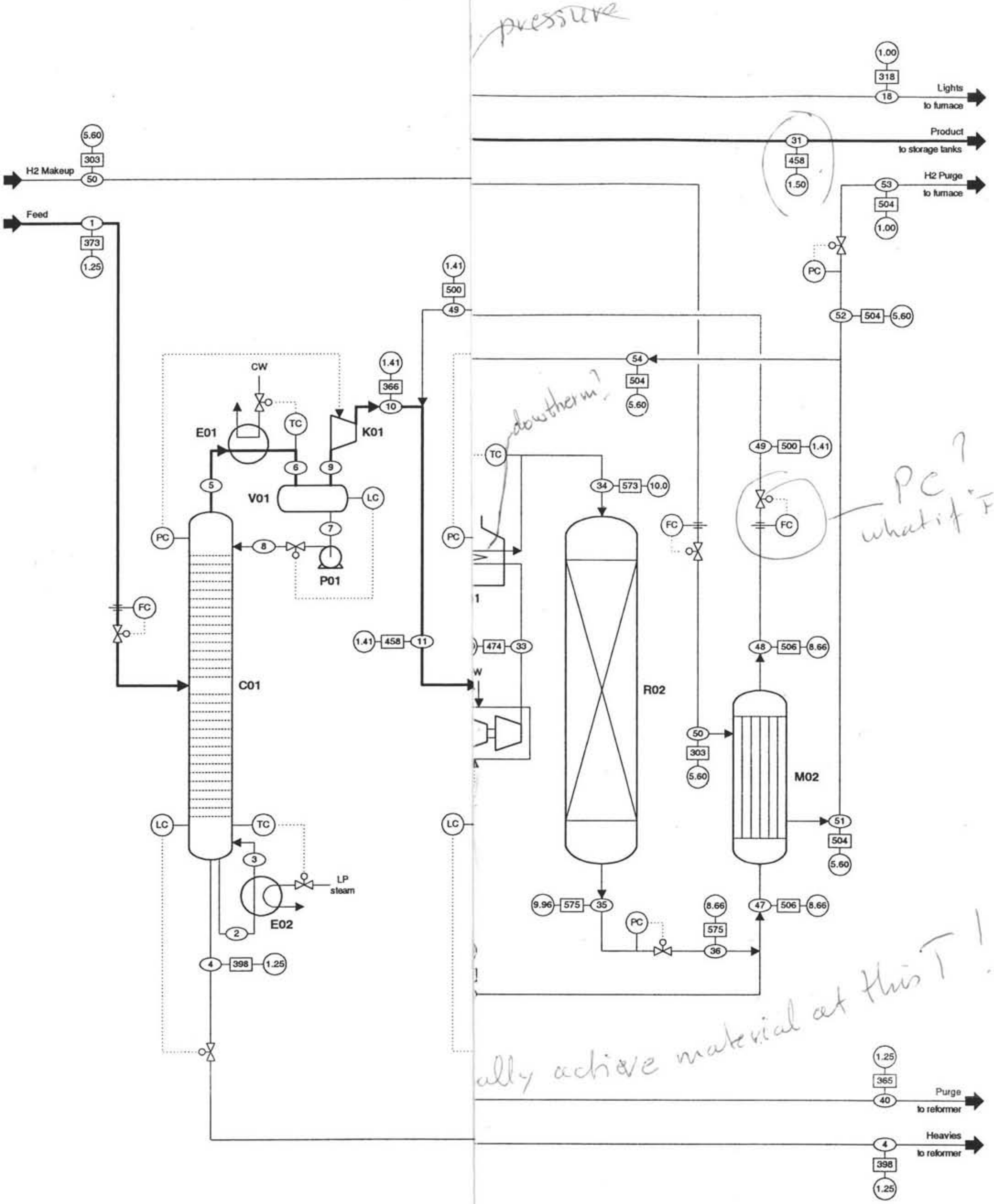
APPENDICES



Process Flow Scheme

C01 : Tailing Column
C02 : Topping Column
C03 : Reactant Separation Column
E01 : Condenser C01
E02 : Reboiler C01
E03 : Condenser C02
E04 : Reboiler C02
E05 : Condenser C03

E06 : Reboiler C03
E07 : Feed Heater R01
E08 : Interstage Cooler
E09 : Interstage Cooler
E10 : Feed Heater M01
E11 : Hydrogen Cooler
E12 : Interstage Cooler
F01 : Feed Heating Fu

ct:	The Hydroisomerization of Heptane (HYHEP)
ct ID number:	CPD3259
pletion Date:	June 19, 2001
on:	20 (Final)
	18/06/01
ame:	PFD20.VSD

ream Number 373 Temperature (K) 1.25 Pressure (bara)

APPENDIX 2: PROCESS STREAM SUMMARY

PROCESS STREAM SUMMARY

STREAM Nr.	:	1		2		3		4		5		6		7		8	
Name	:	raffinate to C01		bottom to E02		after E02		oulet bottom C01		to E01		to V01		liquid from V01		reflux to C01	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/h	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propane	44.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Isobutane	58.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-C6	86.18	129.16	1498.83	0.00	0.00	0.00	0.00	0.00	0.00	313.58	3638.80	313.58	3638.80	184.42	2139.97	184.42	2139.97
2-MP	86.18	56.63	657.09	0.00	0.00	0.00	0.00	0.00	0.00	120.57	1399.09	120.57	1399.09	63.94	741.99	63.94	741.99
3-MP	86.18	52.65	610.99	0.00	0.00	0.00	0.00	0.00	0.00	117.46	1363.04	117.46	1363.04	64.81	752.06	64.81	752.06
N-C7	100.20	193.36	1929.63	15.65	156.16	15.65	156.16	1.35	13.52	834.49	8327.93	834.49	8327.93	642.49	6411.82	642.49	6411.82
2-MHx	100.20	81.37	812.00	0.01	0.08	0.01	0.08	0.00	0.01	292.42	2918.27	292.42	2918.27	211.06	2106.28	211.06	2106.28
3-MHx	100.20	105.28	1050.64	0.04	0.42	0.04	0.42	0.00	0.03	393.17	3923.68	393.17	3923.68	287.89	2873.06	287.89	2873.06
2,2-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DMP	100.20	29.19	291.34	0.00	0.03	0.00	0.03	0.00	0.00	104.71	1044.97	104.71	1044.97	75.52	753.64	75.52	753.64
2,4-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3,3-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-EP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,2,3TMB	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-MHEPT	114.23	104.61	915.76	742.96	6504.04	742.96	6504.04	104.59	915.63	0.11	0.93	0.11	0.93	0.09	0.80	0.09	0.80
3-MHEPT	114.23	82.62	723.25	565.43	4949.92	565.43	4949.92	82.61	723.21	0.04	0.32	0.04	0.32	0.03	0.27	0.03	0.27
4-MHEPT	114.23	33.07	289.48	234.08	2049.16	234.08	2049.16	33.06	289.43	0.03	0.29	0.03	0.29	0.03	0.25	0.03	0.25
2,3-DMHx	114.23	19.50	170.67	145.45	1273.34	145.45	1273.34	19.48	170.56	0.08	0.70	0.08	0.70	0.07	0.59	0.07	0.59
2,4-DMHx	114.23	19.76	172.97	167.57	1466.96	167.57	1466.96	19.24	168.47	2.89	25.29	2.89	25.29	2.37	20.79	2.37	20.79
Total		907.18	9122.64	1871.19	16400.11	1871.19	16400.11	260.35	2280.86	2179.55	22643.29	2179.55	22643.29	1532.72	15801.51	1532.72	15801.51
Enthalpy	kW	-20081		-43020		-36659		-5981		-45543		-51447		-37804		-37804	
Phase		V+L		L		V		L		V		V+L		L		L	
Press.	Bara	1.25		1.25		1.25		1.25		1.01		1.00		1.00		1.00	
Temp	K	373		398		398		398		362		359		359		359	

STREAM Nr.	:	9		10		11		12		13		14		15		16	
Name	:	vapor to K01		top C01 to C02		stream 49 +10		to E04		from E03		to E03		to V02		liquid from V02 to P02	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/h	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propane	44.10	0.00	0.00	0.00	0.00	68.15	1545.34	0.00	0.00	0.00	0.00	162.44	3683.65	162.44	3683.65	94.29	2138.31
Isobutane	58.12	0.00	0.00	0.00	0.00	89.82	1545.37	0.00	0.00	0.00	0.00	372.94	6416.37	372.94	6416.37	283.12	4871.00
N-C6	86.18	129.16	1498.83	129.16	1498.83	143.52	1665.37	54.14	628.25	54.14	628.25	5084.14	58996.54	5084.14	58996.54	4954.98	57497.71
2-MP	86.18	56.63	657.09	56.63	657.09	56.66	657.54	0.18	2.08	0.18	2.08	1668.31	19359.09	1668.31	19359.09	1611.68	18702.00
3-MP	86.18	52.65	610.99	52.65	610.99	52.83	613.10	0.78	9.10	0.78	9.10	1707.75	19816.79	1707.75	19816.79	1655.10	19205.80
N-C7	100.20	192.00	1916.11	192.00	1916.11	446.43	4455.25	767.86	7662.98	767.86	7662.98	0.00	0.02	0.00	0.02	0.00	0.02
2-MHx	100.20	81.36	811.99	81.36	811.99	759.61	7580.62	1646.30	16429.48	1646.30	16429.48	0.38	3.83	0.38	3.83	0.38	3.79
3-MHx	100.20	105.28	1050.61	105.28	1050.61	660.02	6586.75	1361.90	13591.28	1361.90	13591.28	0.12	1.24	0.12	1.24	0.12	1.23
2,2-DMP	100.20	0.00	0.00	0.00	0.00	102.59	1023.81	290.99	2903.98	290.99	2903.98	27.80	277.44	27.80	277.44	27.29	272.32
2,3-DMP	100.20	29.19	291.33	29.19	291.33	295.32	2947.22	639.47	6381.70	639.47	6381.70	0.17	1.74	0.17	1.74	0.17	1.72
2,4-DMP	100.20	0.00	0.00	0.00	0.00	259.98	2594.51	720.20	7187.36	720.20	7187.36	34.31	342.38	34.31	342.38	33.70	336.36
3,3-DMP	100.20	0.00	0.00	0.00	0.00	104.52	1043.05	247.88	2473.72	247.88	2473.72	0.52	5.15	0.52	5.15	0.51	5.07
3-EP	100.20	0.00	0.00	0.00	0.00	63.64	635.10	125.42	1251.63	125.42	1251.63	0.00	0.05	0.00	0.05	0.00	0.05
2,2,3TMB	100.20	0.00	0.00	0.00	0.00	44.58	444.85	120.12	1198.73	120.12	1198.73	4.28	42.72	4.28	42.72	4.21	41.97
2-MHEPT	114.23	0.02	0.13	0.02	0.13	0.76	6.65	0.76	6.64	0.76	6.64	0.00	0.00	0.00	0.00	0.00	0.00
3-MHEPT	114.23	0.00	0.04	0.00	0.04	0.25	2.19	0.24	2.10	0.24	2.10	0.00	0.00	0.00	0.00	0.00	0.00
4-MHEPT	114.23	0.00	0.04	0.00	0.04	0.23	2.05	0.23	2.05	0.23	2.05	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DMHx	114.23	0.01	0.11	0.01	0.11	0.55	4.81	0.59	5.13	0.59	5.13	0.00	0.00	0.00	0.00	0.00	0.00
2,4-DMHx	114.23	0.51	4.50	0.51	4.50	18.64	163.21	23.62	206.77	23.62	206.77	0.00	0.00	0.00	0.00	0.00	0.00
Total		646.83	6841.78	646.83	6841.78	3168.11	33516.80	6000.68	59942.98	6000.68	59942.98	9063.18	108947.03	9063.18	108947.03	8665.56	103077.35
Enthalpy	kW	-13643		-13542		-58476		-146883		-125602		-201989		-240406		-230794	
Phase		V		V		V		L		V		V		V+L		L	
Press.	Bara	1.00		1.41		1.41		1.38		1.38		1.01		1.00		1.00	
Temp	K	359		366		458		374		374		337		318		318	

STREAM Nr. :		17		18		19		20		21		22		23		24	
Name :		reflux from P02 to C02		top C02		bottom C02 to P03		to C03		to E06		from E06		to E05		to V03	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Propane	44.10	94.29	2138.31	68.15	1545.34	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Isobutane	58.12	283.12	4871.00	89.82	1545.37	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-C6	86.18	4954.98	57497.71	129.16	1498.83	14.35	166.54	14.35	166.54	0.00	0.00	0.00	0.00	96.42	1118.89	96.42	1118.89
2-MP	86.18	1611.68	18702.00	56.63	657.09	0.04	0.45	0.04	0.45	0.00	0.00	0.00	0.00	0.26	2.99	0.26	2.99
3-MP	86.18	1655.10	19205.80	52.65	610.99	0.18	2.11	0.18	2.11	0.00	0.00	0.00	0.00	1.22	14.19	1.22	14.19
N-C7	100.20	0.00	0.02	0.00	0.00	446.43	4455.24	446.43	4455.24	1651.78	16484.14	1651.78	16484.14	237.17	2366.86	237.17	2366.86
2-MHx	100.20	0.38	3.79	0.00	0.05	759.60	7580.58	759.60	7580.58	2285.17	22805.16	2285.17	22805.16	2105.35	21010.64	2105.35	21010.64
3-MHx	100.20	0.12	1.23	0.00	0.01	660.02	6586.74	660.02	6586.74	2247.73	22431.51	2247.73	22431.51	1330.31	13276.03	1330.31	13276.03
2,2-DMP	100.20	27.29	272.32	0.51	5.12	102.08	1018.69	102.08	1018.69	3.05	30.46	3.05	30.46	682.81	6814.23	682.81	6814.23
2,3-DMP	100.20	0.17	1.72	0.00	0.02	295.32	2947.20	295.32	2947.20	879.64	8778.51	879.64	8778.51	830.16	8284.70	830.16	8284.70
2,4-DMP	100.20	33.70	336.36	0.60	6.02	259.38	2588.49	259.38	2588.49	17.23	171.97	17.23	171.97	1725.22	17217.04	1725.22	17217.04
3,3-DMP	100.20	0.51	5.07	0.01	0.08	104.51	1042.98	104.51	1042.98	166.44	1660.98	166.44	1660.98	504.06	5030.32	504.06	5030.32
3-EP	100.20	0.00	0.05	0.00	0.00	63.64	635.10	63.64	635.10	230.04	2295.76	230.04	2295.76	94.38	941.91	94.38	941.91
2,2,3TMB	100.20	4.21	41.97	0.08	0.76	44.50	444.09	44.50	444.09	5.58	55.67	5.58	55.67	293.18	2925.85	293.18	2925.85
2-MHEPT	114.23	0.00	0.00	0.00	0.00	0.76	6.65	0.76	6.65	1.73	15.19	1.73	15.19	0.01	0.05	0.01	0.05
3-MHEPT	114.23	0.00	0.00	0.00	0.00	0.25	2.19	0.25	2.19	0.55	4.80	0.55	4.80	0.00	0.01	0.00	0.01
4-MHEPT	114.23	0.00	0.00	0.00	0.00	0.23	2.05	0.23	2.05	0.54	4.69	0.54	4.69	0.00	0.02	0.00	0.02
2,3-DMHx	114.23	0.00	0.00	0.00	0.00	0.55	4.81	0.55	4.81	1.35	11.77	1.35	11.77	0.01	0.06	0.01	0.06
2,4-DMHx	114.23	0.00	0.00	0.00	0.00	18.64	163.21	18.64	163.21	54.32	475.51	54.32	475.51	0.97	8.47	0.97	8.47
Total		8665.56	103077.35	397.62	5869.68	2770.49	27647.12	2770.49	27647.12	7545.14	75226.12	7545.14	75226.12	7901.53	79012.27	7901.53	79012.27
Enthalpy	kW	-230794		-9612		-67540		-67540		-184298		-156856		-169844		-198118	
Phase		L		V		L		L		L		V		V		L	
Press.	Bara	1.00		1.00		1.38		1.38		1.04		1.04		1.00		1.00	
Temp	K	318		318		374		374		367		367		360		359	

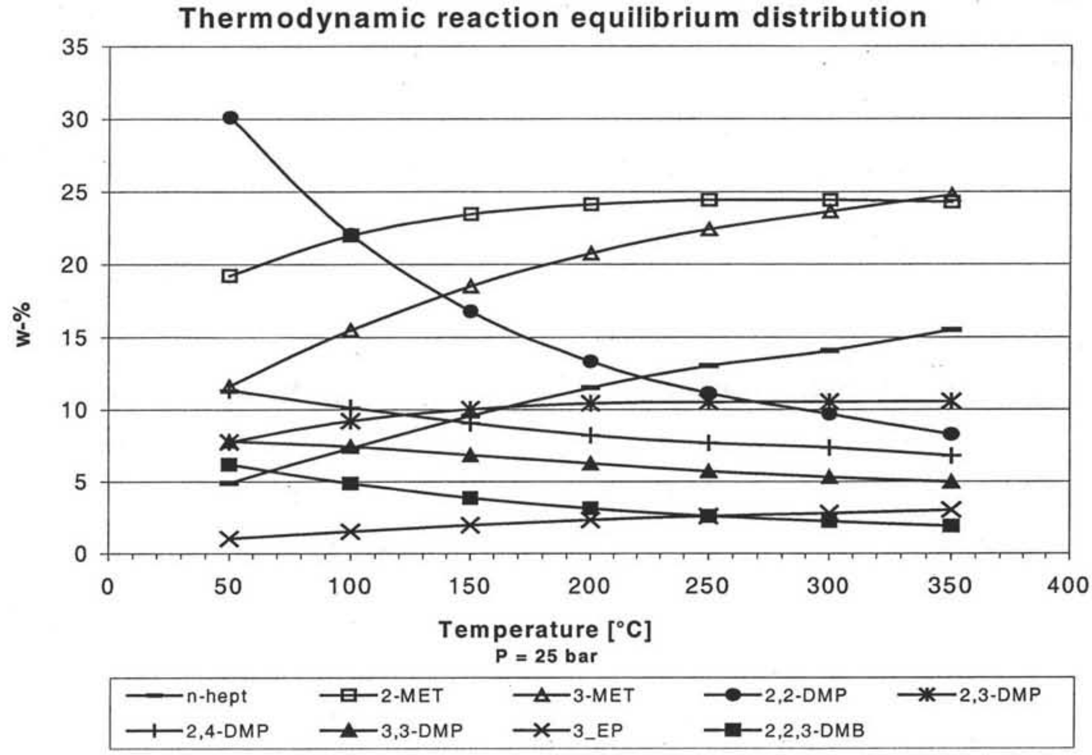
STREAM Nr. :		25		26		27		28		29		30		31		32	
Name :		to P05		to P04		reflux to C03		to E10		to M01		product		product to storage		permeate to K03	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/h	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	77.06	38222.42
Propane	44.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Isobutane	58.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-C6	86.18	14.35	166.54	82.07	952.35	82.07	952.35	14.35	166.54	14.35	166.54	0.00	0.00	0.00	0.00	14.35	166.54
2-MP	86.18	0.04	0.44	0.22	2.55	0.22	2.55	0.04	0.45	0.04	0.45	0.00	0.00	0.00	0.00	0.04	0.44
3-MP	86.18	0.18	2.08	1.04	12.08	1.04	12.08	0.18	2.11	0.18	2.11	0.00	0.00	0.00	0.00	0.18	2.08
N-C7	100.20	35.30	352.29	201.87	2014.57	201.87	2014.57	35.30	352.29	35.30	352.29	0.00	0.00	0.00	0.00	35.30	352.29
2-MHx	100.20	313.36	3127.25	1791.99	17883.39	1791.99	17883.39	313.36	3127.25	313.36	3127.25	0.00	0.00	0.00	0.00	313.36	3127.25
3-MHx	100.20	198.01	1976.02	1132.31	11300.00	1132.31	11300.00	198.01	1976.02	198.01	1976.02	0.00	0.00	0.00	0.00	198.01	1976.02
2,2-DMP	100.20	101.63	1014.24	581.18	5799.99	581.18	5799.99	101.63	1014.24	101.63	1014.24	101.63	1014.24	101.63	1014.24	0.00	0.00
2,3-DMP	100.20	123.56	1233.10	706.60	7051.60	706.60	7051.60	123.56	1233.11	123.56	1233.11	0.00	0.00	0.00	0.00	123.56	1233.10
2,4-DMP	100.20	256.78	2562.60	1468.43	14654.43	1468.43	14654.43	256.78	2562.61	256.78	2562.61	0.00	0.00	0.00	0.00	256.78	2562.60
3,3-DMP	100.20	75.02	748.72	429.03	4281.60	429.03	4281.60	75.02	748.72	75.02	748.72	75.02	748.72	75.02	748.72	0.00	0.00
3-EP	100.20	14.05	140.19	80.33	801.71	80.33	801.71	14.05	140.20	14.05	140.20	0.00	0.00	0.00	0.00	14.05	140.19
2,2,3TMB	100.20	43.64	435.49	249.54	2490.37	249.54	2490.37	43.64	435.49	43.64	435.49	43.64	435.49	43.64	435.49	0.00	0.00
2-MHEPT	114.23	0.00	0.01	0.01	0.04	0.01	0.04	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.01
3-MHEPT	114.23	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4-MHEPT	114.23	0.00	0.00	0.00	0.01	0.00	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2,3-DMHx	114.23	0.00	0.01	0.01	0.06	0.01	0.06	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.00
2,4-DMHx	114.23	0.14	1.26	0.82	7.21	0.82	7.21	0.14	1.26	0.14	1.26	0.14	1.26	0.14	1.26	0.00	0.00
Total		1176.07	11760.23	6725.46	67251.97	6725.46	67251.97	1176.07	11760.29	1176.07	11760.29	220.44	2199.72	220.44	2199.72	1032.69	47782.93
Enthalpy	kW	-29488		-168630		-168630		-29457		-25657		-4413		-4413		-15322	
Phase		L		L		L		L		L		V		V		V	
Press.	Bara	1.00		1.00		1.00		10.00		10.00		10.00		1.50		1.00	
Temp	K	359		359		359		360		458		458		458		473	

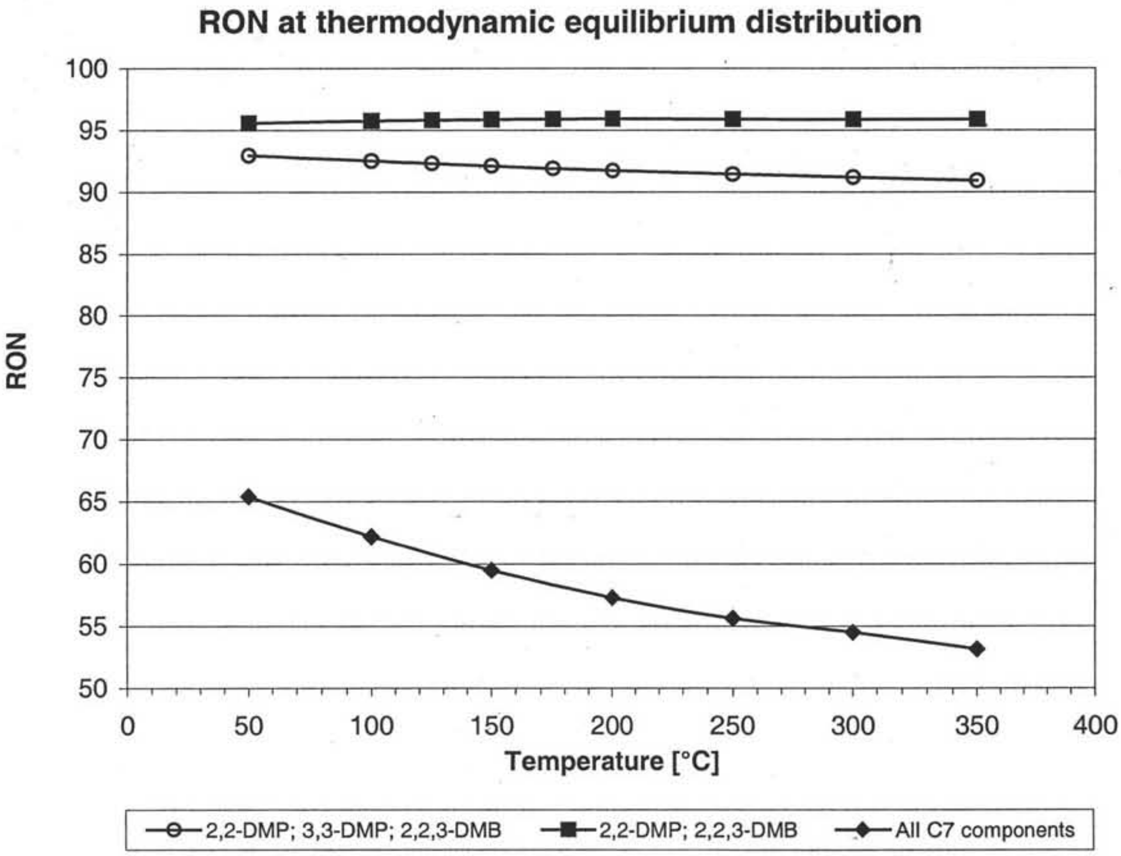
STREAM Nr.	:	33		34		35		36		37		38		39		40	
Name	:	to F01		inlet reactor		outlet reactor to valve		after valve to M02		bottom C03 to P06		after P06		purge to pressure relief		purge	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/h	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	77.06	38222.42	77.06	38222.42	76.81	38102.11	76.81	38102.11	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00
Propane	44.10	0.00	0.00	0.00	0.00	5.31	120.31	5.31	120.31	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00
Isobutane	58.12	0.00	0.00	0.00	0.00	6.99	120.32	6.99	120.32	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00
N-C6	86.18	14.35	166.54	14.35	166.54	14.35	166.54	14.35	166.54	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2-MP	86.18	0.04	0.44	0.04	0.44	0.04	0.45	0.04	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3-MP	86.18	0.18	2.08	0.18	2.08	0.18	2.11	0.18	2.11	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
N-C7	100.20	35.30	352.29	35.30	352.29	47.85	477.52	47.85	477.52	411.13	4102.96	411.13	4102.96	8.22	82.06	8.22	82.06
2-MHx	100.20	313.36	3127.25	313.36	3127.25	299.54	2989.30	299.54	2989.30	446.24	4453.32	446.24	4453.32	8.92	89.07	8.92	89.07
3-MHx	100.20	198.01	1976.02	198.01	1976.02	187.60	1872.21	187.60	1872.21	462.01	4610.72	462.01	4610.72	9.24	92.21	9.24	92.21
2,2-DMP	100.20	0.00	0.00	0.00	0.00	0.06	0.65	0.06	0.65	0.45	4.46	0.45	4.46	0.01	0.09	0.01	0.09
2,3-DMP	100.20	123.56	1233.10	123.56	1233.10	144.46	1441.65	144.46	1441.65	171.76	1714.09	171.76	1714.09	3.44	34.28	3.44	34.28
2,4-DMP	100.20	256.78	2562.60	256.78	2562.60	150.95	1506.44	150.95	1506.44	2.59	25.88	2.59	25.88	0.05	0.52	0.05	0.52
3,3-DMP	100.20	0.00	0.00	0.00	0.00	43.71	436.19	43.71	436.19	29.49	294.26	29.49	294.26	0.59	5.89	0.59	5.89
3-EP	100.20	14.05	140.19	14.05	140.19	16.72	166.89	16.72	166.89	49.59	494.90	0.86	8.60	0.02	0.17	0.99	9.90
2,2,3TMB	100.20	0.00	0.00	0.00	0.00	38.11	380.32	38.11	380.32	0.86	8.60	49.59	494.90	0.99	9.90	0.02	0.17
2-MHEPT	114.23	0.00	0.01	0.00	0.01	0.00	0.01	0.00	0.01	0.76	6.64	0.76	6.64	0.02	0.13	0.02	0.13
3-MHEPT	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.25	2.18	0.25	2.18	0.00	0.04	0.00	0.04
4-MHEPT	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.23	2.05	0.23	2.05	0.00	0.04	0.00	0.04
2,3-DMHx	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.55	4.80	0.55	4.80	0.01	0.10	0.01	0.10
2,4-DMHx	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	18.50	161.95	18.50	161.95	0.37	3.24	0.37	3.24
Total		1032.69	47782.93	1032.69	47782.93	1032.69	47783.00	1032.69	47783.00	1594.41	15886.82	1594.41	15886.82	31.89	317.74	31.89	317.74
Enthalpy	kW	-15317.52		-11107.63		-11108		-11108		-38884		-38845		-777		-777	
Phase		V		V		V		V		L		L		L		L	
Press.	Bara	10.00		10.00		9.96		8.66		1.04		9.50		9.50		1.00	
Temp	K	474		573.2		575		575		367		367		367		365	

STREAM Nr.	:	41		43		44		45		46		47		48		49		50	
Name	:	to E07		feed to R01		H2 to R01		to R1		outlet R01		stream 36+46		outlet M02, retentate		recycle to C02		H2-make-up	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/h	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	0	0.00	0	0.00	250.9763	124492.21	250.98	124492.21	248.10	123067.26	324.92	161169.35	0.00	0.00	0	0.00	3.12	1547.62
Propane	44.10	0	0.00	0	0.00	0	0.00	0.00	0.00	62.84	1425.03	68.15	1545.34	68.15	1545.34	68.145	1545.34	0.00	0.00
Isobutane	58.12	0	0.00	0	0.00	0	0.00	0.00	0.00	82.83	1425.06	89.82	1545.37	89.82	1545.37	89.82158	1545.37	0.00	0.00
N-C6	86.18	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00	0.00	0.00	14.35	166.54	14.35	166.54	14.35163	166.54	0.00	0.00
2-MP	86.18	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00	0.00	0.00	0.04	0.45	0.04	0.45	0.0376929	0.44	0.00	0.00
3-MP	86.18	0.00	0.00	0.00	0.00	0	0.00	0.00	0.00	0.00	0.00	0.18	2.11	0.18	2.11	0.1793636	2.08	0.00	0.00
N-C7	100.20	402.91	4020.90	402.91	4020.90	0	0.00	402.91	4020.90	206.58	2061.61	254.43	2539.13	254.43	2539.13	254.431	2539.13	0.00	0.00
2-MHx	100.20	437.32	4364.25	437.32	4364.25	0	0.00	437.32	4364.25	378.70	3779.34	678.24	6768.63	678.24	6768.63	678.2437	6768.63	0.00	0.00
3-MHx	100.20	452.77	4518.50	452.77	4518.50	0	0.00	452.77	4518.50	367.14	3663.93	554.74	5536.14	554.74	5536.14	554.7433	5536.14	0.00	0.00
2,2-DMP	100.20	0.44	4.37	0.44	4.37	0	0.00	0.44	4.37	102.53	1023.17	102.59	1023.81	102.59	1023.81	102.5902	1023.81	0.00	0.00
2,3-DMP	100.20	168.32	1679.81	168.32	1679.81	0	0.00	168.32	1679.81	121.67	1214.24	266.13	2655.88	266.13	2655.88	266.1297	2655.88	0.00	0.00
2,4-DMP	100.20	2.54	25.37	2.54	25.37	0	0.00	2.54	25.37	109.03	1088.07	259.98	2594.51	259.98	2594.51	259.9798	2594.51	0.00	0.00
3,3-DMP	100.20	28.90	288.37	28.90	288.37	0	0.00	28.90	288.37	60.81	606.87	104.52	1043.05	104.52	1043.05	104.518	1043.05	0.00	0.00
3-EP	100.20	48.60	485.00	48.60	485.00	0	0.00	48.60	485.00	46.92	468.20	63.64	635.10	63.64	635.10	63.63925	635.10	0.00	0.00
2,2,3TMB	100.20	0.85	8.43	0.85	8.43	0	0.00	0.85	8.43	6.47	64.53	44.58	444.85	44.58	444.85	44.57554	444.85	0.00	0.00
2-MHEPT	114.23	0.74	6.51	0.74	6.51	0	0.00	0.74	6.51	0.74	6.51	0.74	6.51	0.74	6.51	0.7439556	6.51	0.00	0.00
3-MHEPT	114.23	0.24	2.14	0.24	2.14	0	0.00	0.24	2.14	0.24	2.14	0.24	2.14	0.24	2.14	0.2447298	2.14	0.00	0.00
4-MHEPT	114.23	0.23	2.01	0.23	2.01	0	0.00	0.23	2.01	0.23	2.01	0.23	2.01	0.23	2.01	0.2298441	2.01	0.00	0.00
2,3-DMHx	114.23	0.54	4.71	0.54	4.71	0	0.00	0.54	4.71	0.54	4.71	0.54	4.71	0.54	4.71	0.5376888	4.71	0.00	0.00
2,4-DMHx	114.23	18.13	158.71	18.13	158.71	0	0.00	18.13	158.71	18.13	158.71	18.13	158.71	18.13	158.71	18.12981	158.71	0.00	0.00
Total		1562.53	15569.08	1562.53	15569.08	250.98	124492.21	1813.50	140061.29	1813.50	140061.39	2846.20	187844.36	2521.28	26675.02	2521.27	26674.95	3.12	1547.62
Enthalpy	kW	-38068		-28599		7589		-21010		-22001		-33108		-44934		-44933			
Phase		L		V		V		V		V		V		V		V		V	
Press.	Bara	9.50		9.50		9.50		9.50		8.66		8.66		8.66		1.41		5.60	
Temp	K	367		473		478		471		473		506		506		500		303	

STREAM Nr. :		51		52		53		54		55		56		57		58	
Name :		permeate M02		H2 purge to PC		H2 purge		H2-recycle		H2 to E11		H2 to K02		H2 recycle to M01		H2 sweep gas for M01	
COMP	MW	tonne/day	kmol/day	tonne/day	kmol/h	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day	tonne/day	kmol/day
Hydrogen	2.02	328.04	162716.96	?	0.00	?	0.00	328.03	162714.63	250.98	124492.21	250.9763	124492.21	77.05639	38222.42	77.05639	38222.42
Propane	44.10	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
Isobutane	58.12	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
N-C6	86.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2-MP	86.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
3-MP	86.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
N-C7	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2-MHx	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
3-MHx	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2,2-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2,3-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2,4-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
3,3-DMP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
3-EP	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2,2,3TMB	100.20	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2-MHEPT	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
3-MHEPT	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
4-MHEPT	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2,3-DMHx	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
2,4-DMHx	114.23	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0	0.00	0	0.00	0	0.00
Total		328.04	162716.96	0.00	0.00	0.00	0.00	328.03	162714.63	250.98	124492.21	250.98	124492.21	77.06	38222.42	77.06	38222.42
Enthalpy	kW	11346		?		?		11327		8666		4109		2661		2661	
Phase		V		V		V		V		V		V		V		V	
Press.	Bara	5.60		5.60		1.00		5.60		5.60		5.60		5.60		1.00	
Temp	K	504		504		504		504		504		396		504		504	

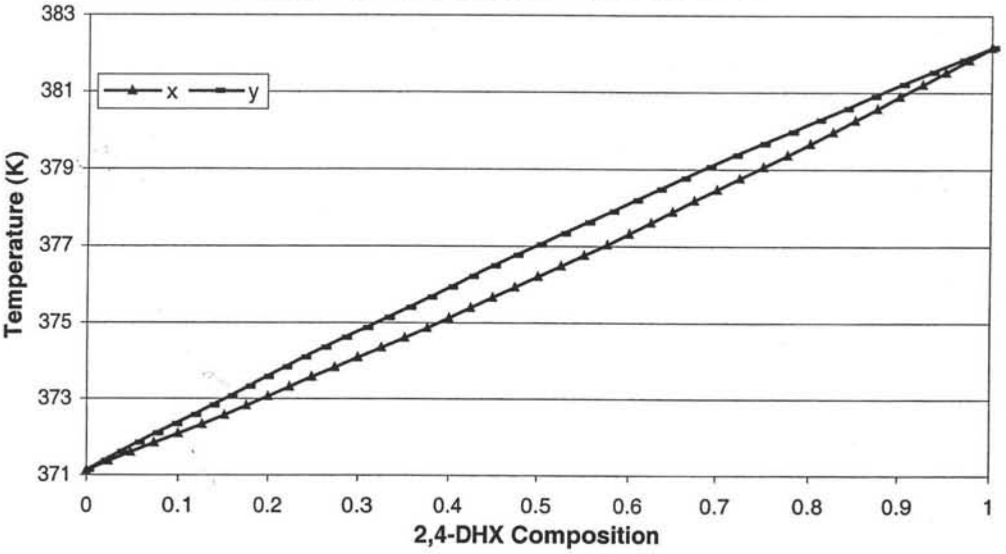
APPENDIX 3: THERMODYNAMIC REACTION EQUILIBRIUM



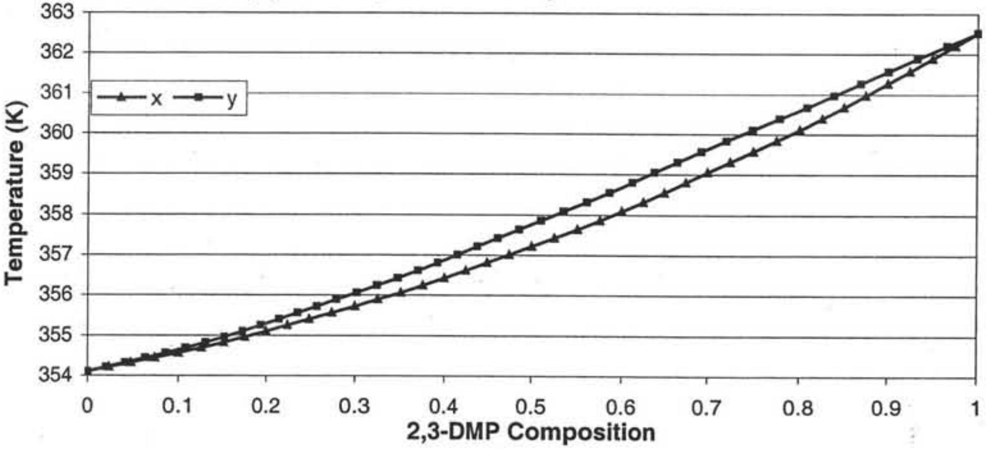


APPENDIX 4: T-XY PLOTS

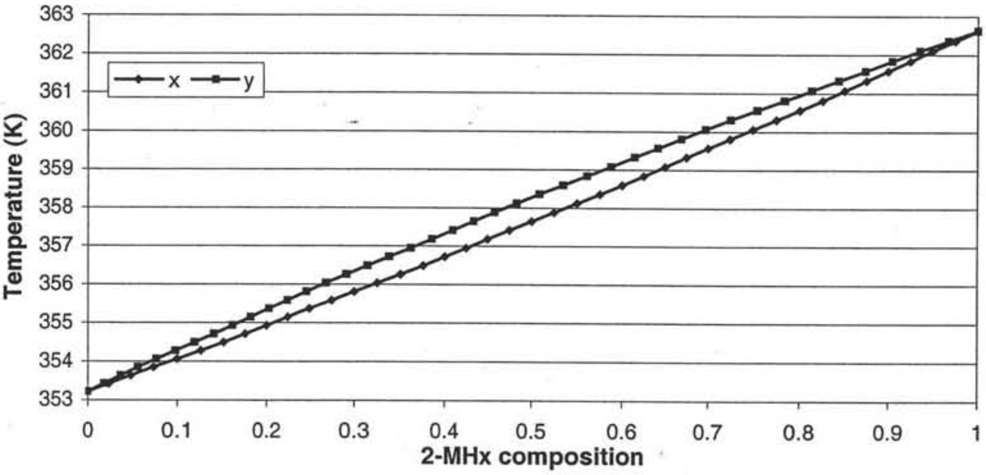
Txy-plot, of n-heptane and 2,4DHX of D1



Txy-plot of 2,3-DMP and cyclohexane of D2



Txy-plot of 2,4-DMP and 2-MHx of D3



APPENDIX 5: THERMODYNAMIC PROPERTIES

(1)=handbook of fysics and chemistry, D.R. Lide
(2)= Yaws
(3)= J.A. Dean Lange's Handbook of Chemistry 14e ed., 1992, USA

	(1) $\Delta_f H^o$ kJ/mol	(2) $\Delta_f G^o$ kJ/mol	(1) S^o J/mol.K	(1) $\Delta_{vap}H$ kJ/mol	(1) T_b K	(1) T_c K	(1) P_c MPa	(1) V_c cm^3/mol	(1) C_P (liq) at 25°C J/mol.K	(1) η (STP) mPa.s
n-C6					341.88	507.6	3.025	368	195.6	
2-MP					333.41	497.7	3.025	368	193.7	
3-MP					336.42	504.6	3.12	368	190.7	
n-C7	-187.6	7.99		31.77	371.7	540.2	2.74	428	224.7	0.387
2-MHx	-194.5	3.22	323.3	30.62	363.19	530.4	2.74	421	222.9	
3-MHx	-191.3	4.6		30.9	365	535.2	2.81	404	221.1	0.35
2,2-DMP	-205.7	0.08	300.3	29.23	352.3	520.5	2.77	416		
2,3-DMP	-198.7	0.67		30.46	362.93	537.3	2.91	393		
2,4-DMP	-201.6	3.1	303.2	29.55	353.64	519.8	2.74	418	224.4	
3,3-DMP	-201.0	2.64		29.62	359.21	536.4	2.95	414		
2,2,3-TMB	-204.4	4.27	292.2	28.9	354.01	531.1	2.95	398	213.5	
3-EP	-189.5	11	314.5	31.12	366.7	540.6	2.89	416	219.6	
2,3-DMHx					388.77	563.5	2.628	468		
2,4-DMHx					382.6	553.6	2.556	472		
2-MHept					390.81	559.7	2.484	488	252	
3-MHept					392.09	563.7	2.546	464	250.2	
4-MHept					390.87	561.8	2.542	476	251.1	
Propane					231	369.8	4.25	203		
Isobutane					261.42	407.9	3.63	257		
Hydrogen					20.28	32.97	1.293	65	28.8 i.g.	

	$\Delta_f G$ 298 K [kJ/kmol]	$\Delta_f G$ 298 K lit 3 [kJ/mol]	rel. dif [%]	$\Delta_f H$ 298 K [kJ/kmol]	$\Delta_f H$ 298 K lit [kJ/mol]	rel.dif [%]	$\Delta_{vap} H$ (T_b) [kJ/kmol]	$\Delta_{vap} H$ (T_b) lit [kJ/mol]	rel. dif [%]	P_c [bar]	P_c lit [MPa]	rel. dif. [%]	T_b [K]	T_b lit [K]	rel. dif. [%]
n-C6	-66			-166940			28786.1			30.25	3.025	0.000	341.88	341.88	0.000
2-MP	-5338			-174550			27884.4			30.40	3.025	0.493	333.41	333.41	0.000
3-MP	-3420			-172000			28260.3			31.20	3.12	0.000	336.42	336.42	0.000
n-C7	8165	8	2.0	-187650	-187.6	0.03	31836.6	31.77	0.21	27.40	2.74	0.000	371.58	371.7	-0.032
2-MHx	3470	3.2	7.8	-194600	-194.5	0.05	30752.5	30.62	0.43	27.40	2.74	0.000	363.20	363.19	0.002
3-MHx	5124	4.6	10.2	-191300	-191.3	0.00	31031.5	30.9	0.42	28.10	2.81	0.000	365.00	365	0.000
2,2-DMP	550	0.1	82.0	-205810	-205.7	0.05	29336.0	29.23	0.36	27.70	2.77	0.000	352.34	352.3	0.011
2,3-DMP	5717	0.7	88.0	-194100	-198.7	-2.37	30486.3	30.46	0.09	29.10	2.91	0.000	362.93	362.93	0.000
2,4DMP	3407	3.1	9.0	-201670	-201.6	0.03	29640.1	29.55	0.30	27.40	2.74	0.000	353.64	353.64	0.001
3,3-DMP	4910	2.6	46.0	-199790	-201.0	-0.61	29737.1	29.62	0.39	29.50	2.95	0.000	359.21	359.21	0.000
2,2,3-TMB	4680	4.3	8.8	-204430	-204.4	0.01	28979.2	28.9	0.27	29.50	2.95	0.000	354.03	354.01	0.006
3-EP	11380	11	3.3	-189330	-189.5	-0.09	31018.7	31.12	-0.33	28.90	2.89	0.000	366.62	366.7	-0.022
2,4-DMHx	11350			-219240			32475.1			25.60	2.556	0.156	382.58	382.6	-0.005
2,3-DMHx	15490			-213800			33180.6			26.30	2.628	0.076	388.76	388.77	-0.003
2-MHept	11690			-215350			33624.3			25.00	2.484	0.640	390.80	390.81	-0.003
4-MHept	15720			-211960			33696.5			25.40	2.542	-0.079	390.86	390.87	-0.003
3-MHept	12757			-212510			33826.2			25.50	2.546	0.157	392.08	392.09	-0.003
Propane	-24390			-104680			18742.7			42.48	4.25	-0.047	231.11	231	0.048
Isobutane	-21440			-134990			21376.8			36.40	3.63	0.275	261.43	261.42	0.004
Hydrogen	0			0			896.5			13.13	1.293	1.523	20.39	20.28	0.539

	Gas							Liquid						
	A	B	C	D	E	C_P (298K) J/mol.K		A	B	C	D	T_{min} [K]	T_{max} [K]	C_P (298K) [J/mol.K]
n-C6	25.924	0.41927	-1.25E-05	-1.26E-07	5.88E-11	146.89		78.848	0.88729	-2.95E-03	3.38E-06	179	457	170.92
2-MP	-7.970	0.60097	3.41E-04	9.52E-08	-1.03E-11	203.83		110.129	0.50521	-1.77E-03	4.20E-06	121	448	214.86
3-MP	-7.123	0.58327	-3.03E-04	6.80E-08	-3.98E-12	141.52		114.18	0.44300	-1.54E-03	2.73E-06	111	454	181.92
n-C7	26.984	0.50387	-4.47E-05	-1.68E-07	6.52E-11	169.22		101.121	0.97739	-3.07E-03	4.18E-06	184	486	230.38
2-MHx	-3.249	0.66250	3.38E-04	6.05E-08	2.54E-12	225.84		118.184	0.71284	-2.31E-03	3.45E-06	156	482	216.50
3-MHx	-12.841	0.71358	-4.20E-04	1.20E-07	-1.29E-12	165.65		126.861	0.64079	-2.06E-03	3.06E-06	155	478	215.85
2,2-DMP	-19.277	0.76888	-5.17E-04	2.05E-07	-3.72E-11	169.08		115.052	0.65770	-2.17E-03	3.33E-06	150	468	206.49
2,3-DMP	38.654	0.37259	2.76E-04	-4.31E-07	1.38E-10	163.89		85.488	0.93200	-2.88E-03	3.76E-06	201	484	206.90
2,4-DMP	-32.996	0.87352	-7.33E-04	3.66E-07	-7.98E-11	171.30		118.526	0.70061	-2.32E-03	3.50E-06	155	468	214.20
3,3-DMP	-23.909	0.78329	-5.40E-04	2.26E-07	-4.43E-11	167.20		118.692	0.60252	-1.93E-03	3.03E-06	140	483	206.75
2,2,3-TMB	-21.150	0.74663	-4.67E-04	1.79E-07	-3.43E-11	164.35		0.826	1.70370	-5.07E-03	5.89E-06	250	478	214.49
3-EP	19.245	0.55072	-1.41E-04	-8.25E-08	3.95E-11	169.01		116.451	0.71000	-2.26E-03	3.35E-06	156	487	215.70
2,3-DMHx	-45.246	0.97100	-7.62E-04	3.49E-07	-7.07E-11	185.17		109.692	1.09000	-3.26E-03	4.15E-06	201	507	255.20
2,4-DMHx	-35.844	0.97300	-7.93E-04	3.81E-07	-8.07E-11	192.97		100.402	1.19520	-3.60E-03	4.65E-06	201	498	259.71
2-MHept	-3.367	0.75824	-3.82E-04	5.74E-08	8.02E-12	190.23		134.965	0.81458	-2.52E-03	3.54E-06	165	504	247.81
3-MHept	-10.106	0.78711	-4.34E-05	9.75E-08	-2.90E-12	223.15		148.156	0.67559	-2.07E-03	3.01E-06	154	507	244.95
4-MHept	-17.581	0.83526	-5.14E-04	1.51E-07	-1.59E-11	189.54		143.202	0.75601	2.34E-03	3.40E-06	217	512	250.87
Propane	28.277	0.11600	1.96E-04	-2.33E-07	6.87E-11	74.63		59.642	0.37831	-1.54E-03	3.65E-06	86	333	
Isobutane	6.772	0.34147	-1.03E-04	-3.68E-08	2.04E-11	98.59		71.791	0.44800	-2.05E-03	4.06E-06	136	383	
Hydrogen	25.399	0.02018	-3.85E-05	3.19E-08	-8.76E-12	28.76								

Literature 3.
$Cp(g) = A+BT+CT^2+DT^3+ET^4$ (T_{min} = 200 K, T_{max} = 1500 K)
$Cp(l) = A+BT+CT^2+DT^3$

Comparison Cp at 1 bar and 298 K from Aspen and from literature

Component	Cp Aspen J/mol.K	Cp Literature J/mol.K	rel.diff. (%)
n-C6	191.69	170.93	10.8
2-MP	189.46	214.95	13.5
3-MP	186.61	181.96	2.5
n-C7	218.06	230.42	5.7
2-MHx	215.44	216.53	0.5
3-Mhx	213.69	215.88	1.0
2,2-DMP	213.69	206.53	3.4
2,3-DMP	208.63	206.93	0.8
2,4-DMP	219.31	214.24	2.3
3,3-DMP	210.81	206.79	1.9
2,2,3-TMB	207.04	214.53	3.6
3-EP	215.02	215.73	0.3
2-MHept	242.48	255.24	5.3
3-MHept	240.30	259.76	8.1
4-MHept	241.44	247.85	2.7
2,3-DMHx	235.97	244.99	3.8
2,4-DMHx	244.55	250.91	2.6

Antoine constants

$$\log P = A - \frac{B}{T+C}$$

P in mm Hg
T in °C
Conversion factor P
1 mm Hg = 0.0013333 bar

log P=A-(B/T+C)	Range		A	B	C	P (25°C) bar
(3)	Tmin (°C)	Tmax (°C)				
n-C6	-9	115	6.8760	1171.17	224.41	0.202
2-MP			6.8391	1135.41	226.57	0.282
3-MP			6.8489	1152.37	227.13	0.253
n-C7			6.8968	1264.90	216.54	0.061
2-MHx	-9	115	6.8732	1236.03	219.55	0.088
3-MHx	-8	117	6.8676	1240.20	219.22	0.082
2,2-DMP	-19	103	6.8148	1190.03	223.30	0.140
2,3-DMP	-10	115	6.8538	1238.02	221.82	0.092
2,4-DMP	-17	105	6.8262	1192.04	225.32	0.155
3,3-DMP	-14	112	6.8267	1228.66	225.32	0.110
2,2,3-TMB			6.7923	1200.56	226.05	0.136
3-EP	-7	119	6.8756	1251.83	219.89	0.077
2,3-DMHx			6.8704	1315.50	214.16	0.031
2,4-DMHx			6.8531	1287.88	214.41	0.040
2-MHept	42	119	6.9174	1337.47	213.69	0.027
3-MHept	43	120	6.8994	1331.53	212.41	0.026
4-MHept			6.9007	1327.66	212.57	0.027
Propane			6.8034	804.00	247.04	9.394
Isobutane			6.9105	946.35	246.88	3.586

APPENDIX 6: FEED COMPOSITIONS

Appendix Table 1: Feedstock IN Battery Limits

Stream Name : <1>			**Raffinate**		
Comp.	Units	Specification			Additional Information
		Available	Design	Notes	(also ref. note numbers)
n-hexane	tonne/day		129.16	1	The original feed is given in
2-methylpentane	tonne/day		56.63		Appendix 6. Table 8:.
3-methylpentane	tonne/day		52.65	2	All comp. with a T_b 20°C higher
n-heptane	tonne/day		193.36		than n-C7 are neglected.
2-methylhexane	tonne/day		81.37	3	All components present less than
3-methylhexane	tonne/day		105.28		0.5 wt % are neglected.
2,3-dimethylpentane	tonne/day		29.19	4	All other cyclic compounds are
2-methylheptane	tonne/day		104.61		neglected, due to the unknown
3-methylheptane	tonne/day		82.62		behaviour in the reactors.
4-methylheptane	tonne/day		33.07		
2,3-dimethylhexane	tonne/day		19.50		
2,4-dimethylhexane	tonne/day		19.76		
Total			100		
Process Conditions and Price					
Temp	°C	100			
Pressure	Bara	1.25			
Phase	V/L/S	V+L			
Price	Nfl/ton	362.08			

Appendix Table 2: Hydrogen make-up In Battery limits

Stream Name : <31>					
Comp.	Units	Specification			Additional Information
		Available	Design	Notes	(also ref. note numbers)
Hydrogen	Tonne/day		3.12		
Total			3.12		
Process Conditions and Price					
Temp.	K	303			
Press.	Bara	5.6			
Phase	V/L/S	L			
Price	Nfl/ton	2000			

Appendix Table 3: Light components OUT of Battery Limits

Stream Name : 18		**Light components**			
Comp.	Units	Specification			Additional Information
		Available	Design	Notes	(also ref. note numbers)
Propane	tonne/day		68.15		
Isobutane	tonne/day		89.15		
N-C6	tonne/day		129.16		
2-MP	tonne/day		56.63		
3-MP	tonne/day		52.65		
2,2-DMP	tonne/day		0.51		
2,4-DMP	tonne/day		0.6		
2,2,3-TMB	tonne/day		0.08		
Total			397.62		
Process Conditions and Price					
Temp.	°C	397.6			
Press.	Bara	1			
Phase	V/L/S	G			
Price	Nfl/ton	315.97			

Appendix Table 4: Heavy components out of Battery Limits

Stream Name : <4>					
Comp.	Units	Specification			Additional Information
		Available	Design	Notes	(also ref. note numbers)
n-C7	tonne/day		1.35		
2-MHx	tonne/day		0.01		
3-MHx	tonne/day		0.04		
2-Mhept	tonne/day		742.96		
3-Mhept	tonne/day		565.43		
4-Mhept	tonne/day		234.08		
2,3-DMHx	tonne/day		145.45		
2,4DMHx	tonne/day		167.57		
Total			260.35		
Process Conditions and Price					
Temp.	°C	398			
Press.	Bara	1.25			
Phase	V/L/S	L			
Price	Nfl/ton	852.05			

Appendix Table 5: Product out of battery limits

Stream Name : <31>					
Comp.	Units	Specification			Additional Information
		Available	Design	Notes	(also ref. note numbers)
2,2-DMP	tonne/day		101.63		
3,3-DMP	tonne/day		75.02		
2,2,3-TMB	tonne/day		43.64		
2,4DMHx	tonne/day		0.14		
Total			220.44		
Process Conditions and Price					
Temp.	°C	458			
Press.	Bara	1.5			
Phase	V/L/S	L			
Price	Nfl/ton	1035.07			

Appendix Table 6: Purge

Stream Name : <40>					
Comp.	Units	Specification			Additional Information
		Available	Design	Notes	(also ref. note numbers)
n-C7	tonne/day		8.22		
2-MHx	tonne/day		8.92		
3-MHx	tonne/day		9.24		
2,2-DMP	tonne/day		0.01		
2,3-DMP	tonne/day		3.44		
2,4-DMP	tonne/day		0.05		
3,3-DMP	tonne/day		0.59		
3-EP	tonne/day		0.02		
2,2,3-TMB	tonne/day		0.99		
2-MHept	tonne/day		0.02		
2,3-DMHx	tonne/day		0.01		
2,4-DMHx	tonne/day		0.37		
Total			31.89		
Process Conditions and Price					
Temp.	°C	365			
Press.	Bara	1			
Phase	V/L/S	L			
Price	Nfl/ton	55.13			

Appendix Table 7:

Original available	100.000 wt %
Components with Tb > 20°C then n-C7	-53.830 wt %
Components which are present less than 0.5 wt %	-11.756 wt %
Cyclic components	-13.780 wt %
Design feed	20.634 wt %

Appendix 6. Table 8: Original feed

Compound	wt%	Compound	wt%	Compound	wt%	Compound	wt%
c5		1c,2t,3-trimethylcyclopentane	1.74	N20	0.29		
i-pentane	0.11	1t,4-dimethylcyclohexane	0.51	I9	0.09		
n-pentane	0.42	1,1-dimethylcyclohexane	0.19	i-butylcyclopentane	0.17	I21	0.05
cyclopentane	0.16	3c-ethylmethylcyclopentane	0.45	n-nonane	4.52	I22	0.05
c6		3t-ethylmethylcyclopentane	0.38	1,1-methylethylcyclohexane	0.35	N37	0.07
2,2-dimethylbutane	0.06	2t-ethylmethylcyclopentane	0.65	N24	0.05	i-butylbenzene	0.07
2,3-dimethylbutane	0.31	1,1-methylethylcyclopentane	0.05	N25	0.06	I25	0.09
2-methylpentane	1.80	1t,2-dimethylcyclohexane	0.62	i-propylbenzene	0.17	sec-butylbenzene	0.04
3-methylpentane	1.67	1t,3-dimethylcyclohexane	0.81	N27	0.37	n-decane	1.71
n-hexane	4.10	n-octane	5.64	i-propylcyclohexane	0.14	1,3-methyl-i-propylbenzene	0.09
methylcyclopentane	1.66	i-propylcyclopentane	0.17	N29	0.06	1,4-methyl-i-propylbenzene	0.07
benzene	0.24	N2	0.15	n-butylcyclopentane	0.31	sec-butylcyclohexane	0.05
cyclohexane	1.18	N3	0.05	n-propylbenzene	0.43	1,2-methyl-i-propylbenzene	0.24
c7		1c,2-dimethylcyclohexane	0.57	1,3-methylethylbenzene	1.03	1,3-diethylbenzene	0.09
2,2-dimethylpentane	0.07	N4	0.98	1,4-methylethylbenzene	0.51	1,3-methyl-n-propylbenzene	0.10
2,4-dimethylpentane	0.26	ethylcyclohexane	0.16	1,3,5-trimethylbenzene	0.19	1,4-methyl-n-propylbenzene	0.05
3,3-dimethylpentane	0.06	n-propylcyclopentane	0.12	1,2-methylethylbenzene	0.57	n-butylbenzene	0.06
2-methylhexane	2.58	ethylbenzene	1.02	1,2,4-trimethylbenzene	1.21	1,3-dimethyl-5-ethylbenzene	0.07
2,3-dimethylpentane	0.93	1,3-dimethylbenzene	2.81	1,2,3-trimethylbenzene	0.26	1,2-diethylbenzene	0.04
1,1-dimethylcyclopentane	0.20	1,4-dimethylbenzene	1.19	2-3-dihydroindene	0.11	1,4,dimethyl-2-ethylbenzene	0.06
3-methylhexane	3.34	1,2-dimethylbenzene	1.83	**c10**		A3	0.13
1c,3-dimethylcyclopentane	0.83	**c9**		I12	0.17	**c11**	
1t,3-dimethylcyclopentane	0.76	2,3,4-trimethylhexane	0.06	2,4-dimethyloctane	0.25	I30	0.11
3-ethylpentane	0.29	1,1,4-trimethylcyclohexane	1.53	2,6-dimethyloctane	0.52	I31	0.17
1t,2-dimethylcyclopentane	1.19	2,2,3-trimethylhexane	0.07	2,5-dimethyloctane	0.30	I32	0.07
n-heptane	6.13	2,4-dimethylheptane	0.94	N30	0.15	I33	0.08

Appendix Table 9: Original feed (continued)

Compound	wt%	Compound	wt%	Compound	wt%	Compound	wt%
methylcyclohexane	3.93	4,4-dimethylheptane	0.89	I14	0.06	N41	0.11
ethylcyclopentane	0.77	2,5-dimethylheptane	0.19	3,3-dimethyloctane	0.96	I37	0.07
toluene	2.27	3,3-dimethylheptane	0.12	N31	0.08	I38	0.06
2,2,3-trimethylhexane		N11	0.37	3,6-dimethyloctane	0.24	I40	0.13
c8		1c,2t,4t-trimethylcyclohexane	0.33	3-methyl-5-ethylheptane	0.45	n-undecane	0.22
1,1,3-trimethylcyclopentane	0.38	I3	0.08	N32	0.09		
2,5-dimethylhexane	0.45	2,3-dimethylheptane	0.67	2,3-dimethyloctane	0.62		
2,4-dimethylhexane	0.63	3,4-dimethylheptane	0.07	I15	0.20		
1c,2t,4-trimethylcyclopentane	0.58	N14	0.21	N34	0.08		
3,3-dimethylhexane	0.08	I5	0.29	I16	0.20		
1t,2c,3-trimethylcyclopentane	0.61	4-methyloctane	1.12	5-methylnonane	0.58		
2,3,4-trimethylpentane	0.10	2-methyloctane	1.38	I17	0.46		
2,3-dimethylhexane	0.62	N15	0.12	2-methylnonane	0.06		
2-methyl-3-ethylpentane	0.23	3-ethylheptane	0.41	3-ethyloctane	0.11		
2-methylheptane	3.32	3-methyloctane	1.88	N35	0.06		
4-methylheptane	1.05	1,1,2-trimethylcyclohexane	0.06	3-methylnonane	0.59		
3,4-dimethylhexane	0.20	I6	0.05	N36	0.06		
1c,3-dimethylcyclohexane	0.18	N18	0.49	I20	0.12		
3-methylheptane	2.62	N19	0.54	i-butylcyclohexane	0.24		

APPENDIX 7: BALANCE FOR STREAM COMPONENTS AROUND THE BATTERY LIMIT

	In		Out				Out-in
Stream nr.	1	50	4	18	40	31	
Stream	Feed	H2- make-up	Heavy comp.	Light comp	purge	product	
	tonne/day	tonne/day	tonne/day	tonne/day	tonne/day	tonne/day	tonne/day
Hydrogen	0.00	3.12	0.00	0.00	0.00	0.00	-3.12
Propane	0.00	0.00	0.00	68.15	0.00	0.00	68.15
Isobutane	0.00	0.00	0.00	89.82	0.00	0.00	89.82
n-C6	129.16	0.00	0.00	129.16	0.00	0.00	0.00
2-MP	56.63	0.00	0.00	56.63	0.00	0.00	0.00
3-MP	52.65	0.00	0.00	52.65	0.00	0.00	0.00
n-C7	193.36	0.00	1.35	0.00	8.22	0.00	-183.78
2-MHx	81.37	0.00	0.00	0.00	8.92	0.00	-72.44
3-MHx	105.28	0.00	0.00	0.00	9.24	0.00	-96.03
2,2-DMP	0.00	0.00	0.00	0.51	0.01	101.63	102.15
2,3-DMP	29.19	0.00	0.00	0.00	3.44	0.00	-25.76
2,4-DMP	0.00	0.00	0.00	0.60	0.05	0.00	0.66
3,3-DMP	0.00	0.00	0.00	0.01	0.59	75.02	75.62
2,2,3-TMB	0.00	0.00	0.00	0.08	0.02	43.64	43.73
3-EP	0.00	0.00	0.00	0.00	0.99	0.00	0.99
2-MHept	104.61	0.00	104.59	0.00	0.02	0.00	0.00
3-MHept	82.62	0.00	82.61	0.00	0.00	0.00	0.00
4-MHept	33.07	0.00	33.06	0.00	0.00	0.00	0.00
2,3-DMHx	19.50	0.00	19.48	0.00	0.01	0.00	0.00
2,4-DMHx	19.76	0.00	19.24	0.00	0.37	0.14	0.00
Total Flow	907.183	3.115	260.353	397.619	31.888	220.438	-7.09E-06
Temperature K	373.15	504.15	397.92	318.30	366.74	458.15	
Pressure Bar	1.25	5.6	1.25	1	1.04	10.0	
Vapor Frac	0.59	1.00	0.00	1.00	0.00	1.00	
Liquid Frac	0.41	0.00	1.00	0.00	1.00	0.00	
Enthalpy kW	-20081	-20	-5981	-9612	-777	-4413	-683
Average MW	99.44	2.02	114.15	67.74	100.36	100.21	

APPENDIX 8: TOTAL MASS STREAMS SUMMARY

HEAT & MASS BALANCE FOR STREAMS TOTAL										
IN						OUT				
Plant		EQUIPMENT			EQUIPM.	EQUIPMENT			Plant	
Mass tonne/day	Heat kW	Mass tonne/day	Heat KW	Stream Nr.	IDENTIF.	Stream Nr.	Mass tonne/day	Heat kW	Mass tonne/day	Heat kW
		907.1827	-20081	**1**	**C01**	**9**	646.8301	-13642.7		
						4	260.3526	-5980.61		
	457	907.18	-20081		Total		907.18	-19623		
		646.83	-13643	**9**	**K01**	**10**	646.8301	-13542		
	101	646.83	-13643		Total		646.83	-13542		
		3168.11	-58476	**11**	**C02**	**18**	397.6187	-9612		
						19	2770.489	-67540		
		3168.11	-58476		Total		3168.11	-77153		18677
		2770.489	-67540	**20**	**C03**	**37**	1594.415	-38884		
						25	1176.074	-29488		
		2770.49	-67540		Total		2770.49	-68372		832
		1594.415	-38884	**37**	**P06**	**38**	1594.415	-38845		
	39	1594.41	-38884		Total		1594.41	-38845		
		250.98	4109	**56**	**K02**	**44**	250.9763	7589		
	3480	250.98	4109		Total		250.98	7589		
		1813.01	-21010	**45**	**R01**	**46**	1813.011	-22001		
		1813.01	-21010		Total		1813.01	-22001		991
		1176.074	-29488	**25**	**P05**	**28**	1176.074	-29457		
	32	1176.07	-29488		Total		1176.07	-29457		
		1176.074	-29457	**28**	**E10**	**29**	1176.074	-25657		
	3800	1176.07	-29457		Total		1176.07	-25657		
		1176.074	-25657	**29**	**M01**	**30**	220.4383	-4413		
		77.06	2661	**58**		**32**	1032.692	-15322		
	3260	1253.13	-22996		Total		1253.13	-19735		
		1032.69	-15322	**32**	**K03+E12**	**33**	1032.692	-15318		
	5	1032.69	-15322		Total		1032.69	-15318		
		1032.692	-15318	**33**	**F01**	**34**	1032.69	-11108		
	4210	1032.69	-15318		Total		1032.69	-11108		
		1032.692	-11108	**34**	**R02**	**35**	1032.692	-11108		
		1032.69	-11108		Total		1032.69	-11108		
		1032.692	-11108	**35**	**pc**	**36**	1032.692	-11108		
		1032.69	-11108		Total		1032.69	-11108		
		2846.195	-33108	**47**	**M02**	**48**	2521.278	-44934		
		3.12		**50**		**51**	328.04	11346		
		2846.20	-33108		Total		2849.32	-33587		479
		250.98	8666	**55**	**E11**	**56**	250.98	4109		
		250.98	8666		Total		250.98	4109		4557
		1562.53	-38068	**41**	**E07**	**43**	1562.53	-28599		
	9469	1562.53	-38068		Total		1562.53	-28599		
	24852				Total					**25535**
									6.5E-03	**683**

Project ID Number :	**CPD3259**
Completion Date :	19 June 2001

APPENDIX 9: SUMMARY OF UTILITIES

SUMMARY OF UTILITIES

EQUIPMENT		UTILITIES													REMARKS
		Heating					Cooling				Power				
		Load	Consumption (t/d)				Load	Consumption (t/d)			Actual Load	Consumption (t/d, kWh/h)			
			Steam		Fuel	Hot Oil		Cooling Water	Air	Refrig.		Steam (t/h)		Electr.	
Nr.	Name	kW	LP	HP			kW				kW	HP	MP	kWh/h	
E01	Condensor C01						-5904	6156							
E02	Reboiler C01	6361	240												
E03	Condensor C02						-39841	57673							
E04	Reboiler C02	21164	803												
E05	Condensor C03						-28274	29261							
E06	Reboiler C03	27443	1038												
E07	preheater HC R01 feed	9478		380											
E08	1st interstage cooler R01						-495								
E09	2nd interstage cooler R01						-495								
E10	membrane feed heater'	3800		152											
E11	Hydrogen cooler						-4108	4710							
E12A	intercooler compressor						-1978	2053							
E12B	intercooler compressor						-2046	2114							
E12C	intercooler compressor						-2011	2081							
F01	Heating furnace R02	6242			14										
P01	reflux pump C01										6			6	
P02	reflux pump C02										52			52	
P03	feed C03 pump										13			13	
P04	reflux pump C03										39			39	
P05	membrane feed pump										32			32	
P06	bottom C03 pump										39			39	
K01	feed C02 compressor										112			112	
K02	hydrogen to R01 compressor										3867			3867	
K03	R02 feed compressor										6667			6667	
TOTAL		68246	**2082**	**532**	14		-85152	**104048**			10827			**10827**	

Designers:	M.A. Rijkse V. Tjon Soei Len	E.S.E.D. van Kints B.M. Vogelaar	Project ID Number: Completion Date :	**CPD 3259** 19th June 2001

APPENDIX 10: PROCESS YIELDS

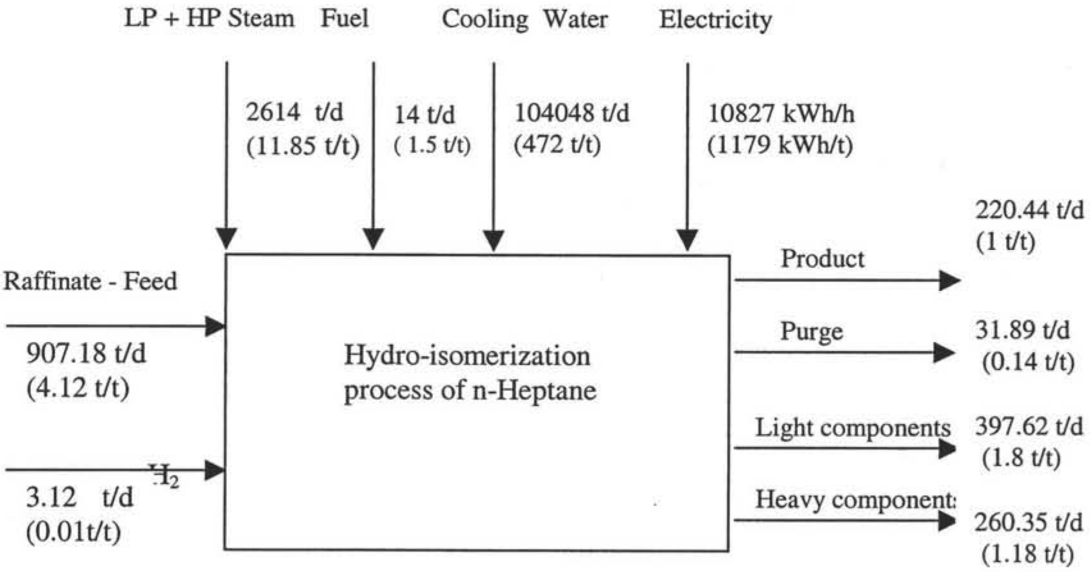
PROCESS YIELDS

Process Streams

Name	Ref. Stream	tonne/day IN	tonne/day OUT	t/h IN	t/h OUT	t/t product IN	t/t product OUT
Raffinate Feed	1	907.18		37.799		4.12	
hydrogen	50	3.12		0.130		0.01	
product	31		220.44		9.19		**1.00**
purge	40		31.89		1.33		0.14
light	18		397.62		16.57		1.80
heavy	4		260.35		10.85		1.18
Total		910.30	910.30	37.929	37.929	4.13	4.13

Utilities

Name	Ref. Stream	tonne/day	kW	t/h	kWh/h	t/t product	kWh/ t product
LP Steam	-	2082		87		9.44	
HP Steam	-	532		22		2.41	
CW	-	104048		4335		472.00	
Electricity	-		10827		10827		1178.77
Fuel		14		0.58		1.52	



APPENDIX 11: DESCRIPTION OF THE ASPEN SIMULATION

Incoming streams

The process has two feed streams, one is the raffinate coming from the hydrotreater, and the other is the hydrogen make-up.
The raffinate is entering with a temperature of 373 K and a pressure of 1.25 bara, with the composition of the design feed which is given in chapter 3.
The make-up hydrogen that is used for both reactors and the membrane is supplied at 200°C and 1 bara.

Separation section

Distillation columns
The raffinate enters the first distillation column, to separate the C6 and C7 fraction from the heavier compounds. In the design two key components are used, the light key is n-C7 and the heavy key is 2,4-DMHx, recovery in the distillate are respectively 0.993 and 0.026. The bottom stream is then mixed with a recycle stream and goes to the second distillation column.
The second column separates the light components from the C7-fraction. The light key component is n-C6 and the heavy key is 2,2-DMP, the distillate recoveries are respectively 0.9 and 0.005. The third distillation column separates the C7-fraction, the light key component is 2,4-DMP and the heavy key is 3-MHx, the distillate recoveries are respectively 0.99 and 0.3.
The recycle composition is estimated, with the literature conversion data, since the reactors are not yet simulated. This is necessary, because 2,2-DMP (a key component) is not available in the feed.
The number of trays, the feedstage and the reflux ratio of the three distillation columns are first estimated with a shortcut model DSTWU.

With the results of the DSTWU model a RADFRAC model replaces the DSTWU model. Design specifications are used to obtain the desired separation, when streams varies during the design. The design specification is to obtain a desired purity of the light and heavy key component, which can be realised by adapting the reflux ratio and the distillate to feed ratio.
With the model "TraySizing" and "TrayRating" in Radfrac also the dimensions of the columns are calculated. The most important results are the pressure drop per stage and the column diameter.
To obtain pressures that are not below 1 bar use is made of compressors and pumps.

Membranes
A simple SEP model is used for the membranes. This model separates the incoming streams according to the splitfactors given with a known pressure drop. The real design of the membranes is calculated with Excel.
The reaction section

Now there is a feed for both reactors. The reactors are modelled with Rplug. The first reactor is isothermal operated, while the second is operated adiabatically.
The reaction kinetics is used from the modelling described in Chapter 8.2.2.
The temperatures are 473K in the first reactor and 573K, because questions would arise of "how realistic is the simulation?", when the temperatures would deviate too much from the experimental data.
A model optimisation is used to calculate the pressure and dimensions of both reactors to obtain a high conversion to 2,4DMP in the first reactor and the largest possible product stream.

Some constraints were necessary, because Aspen calculated an infinite reactor. These constrains were a maximum length of 15 meter a maximum diameter of 5 meter, a maximum pressure of 10 bars and a maximum recycle stream of 3 times the feed stream. Higher values would make the process too expensive, by catalyst costs, or energy consumption.
This optimisation gave the results in Appendix Table 10 .

Appendix Table 10: Results reactor optimisation

	Reactor 1	Reactor 2
Length [m]	14	14
Diameter [m]	3.7	4.3
Pressure [m]	9.5	10

Compressors
The compressors have a maximum pressure ratio of 3. Therefore compressor C102 must be a three-staged compressor with each stage a pressure ratio of 2.15. The other compressors can be single stage, since the pressure ratio is lower than 3.
The compressors are isentropic with an isentropic efficiency of 0.72 and a mechanical efficiency 1.0.

APPENDIX 12: COLUMN SIZING CALCULATIONS

Theory

Here all equations that were used to calculate all column properties are summed up, together with a detailed description of the calculation procedure.

Diameter

The diameter has to be calculated for the rectifying section (top) and the stripping section (bottom). Different diameters can be chosen for top and bottom, but in this design the diameters for rectifying and stripping section do not differ a lot, so the largest column diameter is chosen. The flooding condition fixes the upper limit of the vapor velocity. Flooding fld [-] is taken as 85% for design.

The flooding velocity u_f [m/s] can be estimated from the correlation of Fair:

$$u_f = K_{1,corrected} \bullet \sqrt{\frac{\rho_L - \rho_V}{\rho_v}} \tag{0.1 }$$

where: K_1 = constant obtained from Fig. 11.27 in C&R [-]
ρ_V = vapor density [kg/m^3]
ρ_L = liquid density [kg/m^3]

To obtain K_1 from Fig. 11.27 [24] the liquid-vapor factor F_{LV} [-] needs to be calculated:

$$F_{LV} = \frac{L_m}{V_m} \bullet \sqrt{\frac{\rho_V}{\rho_L}} \tag{0.2}$$

where: L_m = liquid mole flow rate [kmole/h]
V_m = vapor mole flow rate [kmole/h]

With the calculated liquid-vapor factor F_{LV} and the trial tray spacing (t_s) set at t_s=0.5 m, K_1 can be obtained from Fig. 11.27 in [24].

The constant K_1 might need to be corrected using the equation:

$$K_{1,corrected} = K_1 \bullet \left(\frac{\sigma}{0.02}\right)^{0.2} \tag{0.3}$$

where: σ = surface tension [N/m]

The maximum vapor velocity u_v [m/s] at the flooding estimate is:

$$u_v = u_f \bullet \frac{fld}{100} \tag{0.4}$$

where: fld = flooding, take 85% for design [%]

To calculate the column diameter an estimate has to be made about the downcomer area. Typically, a first estimate of the downcomer area is taken as 12% of the total column area:

$$\alpha = \frac{A_d}{A_c} \cdot 100 \tag{0.5}$$

where: $\alpha =$ downcomer area A_d as percentage of total column area A_c [%]
$A_d =$ downcomer area [m^2]
$A_c =$ total column cross-sectional area [m^2]

The net area A_n [m^2] available for vapor-liquid disengagement, normally equal to (A_c-A_d) for a single pass plate, is:

$$A_n = \frac{\Phi_{v,\max}}{u_v} \tag{0.6}$$

where: $\Phi_{V,\max} =$ maximum volumetric vapor flow rate [m^3/s]

The maximum volumetric vapor flow rate $\Phi_{V,\max}$ [m^3/s] can be calculated:

$$\Phi_{v,\max} = \frac{V_m \cdot MW_V}{\rho_V \cdot 3600} \tag{0.7}$$

where: $MW_V =$ molecular weight vapor [g/mol]

Total cross sectional area of the column A_c [m^2] is:

$$A_c = \frac{A_n}{(1 - \frac{\alpha}{100})} \tag{0.8}$$

Finally, the column diameter D_c [m] can be calculated:

$$D_c = \sqrt{\frac{4 \cdot A_c}{\pi}} \tag{0.9}$$

Liquid flow pattern

The liquid flow pattern will depend on the liquid flow rate, the diameter of the column and the plate type (single pass, double pass, etc.).

Calculate the maximum volumetric liquid flow rate $\Phi_{L,\max}$ [m^3/s]:

$$\Phi_{L,\max} = \frac{L_m \cdot MW_L}{\rho_L \cdot 3600} \tag{0.10}$$

where: MW_L = molecular weight liquid [g/mol]

From Fig. 11.28 in [24], based on the volumetric flow rate $\Phi_{L,max}$ and the column diameter D_c, a choice can be made for selection of the flow arrangement.

Weeping

The minimum vapor velocity is set by the weeppoint. The minimum design vapor velocity $u_{h,min}$ [m/s] is given by:

$$u_{h,\min} = \frac{K_2 - 0.9 \bullet (25.4 - D_h)}{\sqrt{\rho_V}} \tag{0.11}$$

where: K_2 = constant obtained from Fig. 11.30 C&R [-]
D_h = hole diameter [m]

The hole diameter D_h is arbitrarily set in the provisional plate design, usually between 2.5 and 12 mm and typically 5 mm. To obtain K_2 from Fig 11.30 in [24], one has to calculate the clear liquid depth (h_w+h_{ow}) [mm]. The weir height h_w is set at the provisional plate design.

The minimum height of the liquid crest over the downcomer weir is:

$$h_{ow,\min} = 750 \bullet \left(\frac{\Phi_{L,\min}}{\rho_L \bullet l_w} \right)^{\frac{2}{3}} \tag{0.12}$$

where: $\Phi_{L,min}$ = minimum liquid rate at 70% turn-down [kg/s]
l_w = weir length [m]

The minimum liquid rate $\Phi_{L,min}$ [kg/s] is calculated:

$$\Phi_{L,\min} = \Phi_{L,\max} \bullet 0.70 = \frac{L_m \bullet MW_L}{3600} \bullet 0.70 \tag{0.13}$$

Plate pressure drop

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

$$h_t = h_d + (h_w + h_{ow}) + h_r \tag{0.14}$$

where: h_d = dry plate pressure drop [mm]
(h_w+h_{ow}) = clear liquid depth [mm]
h_r = residual head [mm]

The dry plate drop h_d [mm] is:

$$h_d = 51 \cdot \left(\frac{u_{h,\max}}{C_0} \right)^2 \cdot \left(\frac{\rho_V}{\rho_L} \right) \tag{0.15}$$

where:		
$u_{h,\max}$ =	maximum vapor velocity through holes	[m/s]
C_0 =	orifice coefficient, obtained from Fig. 11.34 C&R	[-]

The residual head h_r [mm] is given by:

$$h_r = \frac{12500}{\rho_L} \tag{0.16}$$

Finally, the pressure difference per plate $\Delta P_{tot,plate}$ [Pa] can be calculated:

$$\Delta P_{tot,plate} = 9.81 \cdot h_t \cdot 0.001 \cdot \rho_L \tag{0.17}$$

Downcomer back up

The level of the liquid and froth in the downcomer needs to be well below the top of the outlet weir at the plate above.

The height of liquid backed up in the downcomer h_b [mm liquid] is:

$$h_b = (h_w + h_{ow}) + h_t + h_{dc} \tag{0.18}$$

where:		
(h_w+h_{ow}) =	clear liquid depth	[mm liquid]
h_t =	total pressure drop	[mm liquid]
h_{dc} =	head loss in downcomer	[mm liquid]

The head loss in the downcomer can be estimated with:

$$h_{dc} = 166 \cdot \left(\frac{L_m \cdot MW_L}{\rho_L \cdot A_m \cdot 3600} \right)^2 \tag{0.19}$$

where: A_m = clearance area under the downcomer, equivalent to A_{ap} [m^2]

The height of the clear liquid back up in the downcomer h_b should to be less than half the tray spacing t_s:

$$h_b < 0.5 \cdot (t_s + h_w \cdot 0.001) \tag{0.20}$$

where:		
t_s =	tray spacing	[m]
h_w =	weir height	[mm]

Downcomer residence time

The downcomer residence time needs to be at least 3 seconds to allow the vapor to disengage from the liquid in the downcomer. The residence time t_r is calculated by:

$$t_r = \frac{A_d \bullet h_b \bullet \rho_L}{L_m \bullet MW_L} * 3600 \tag{0.21}$$

Entrainment

Flooding fld [%] is calculated by:

$$fld = \frac{u_{V,act}}{u_f} \bullet 100 \tag{0.22}$$

where: $u_{v,act}$ = actual vapor velocity, based on net area A_n [m/s]
u_f = flooding vapor velocity, as calculated earlier [m/s]

This percentage should be checked with the initial flooding estimate of 85%. If the calculated flooding is lower, the column diameter D_c can be reduced, which will increase the pressure drop.

Example: C01-Rectifying (top) section

Because liquid and vapor flow rates and compositions vary up the column, the design should be made above and below the feed point. Only the rectifying section (top) will be designed in detail in this example.

Physical data from Aspen Plus:

Property	**Description**	**Value for top section**	**Value for bottom section**	**Unit**
Vm	Vapor mole flow rate	840.61	419.22	kmole/h
Lm	Liquid mole flow rate	554.64	514.14	kmole/h
ρ_V	Vapor density	3.304	3.680	kg/m^3
ρ_L	Liquid density	553.55	547.22	kg/m^3
σ	Surface tension	0.0131	0.0122	N/m
MW_V	Molecular weight vapor	94.57	113.95	g/mole
MW_L	Molecular weight liquid	97.06	114.06	g/mole

Column diameter:

Starting estimates:

Formula/Symbol	**Description**	**Value**	**Unit**
ts	Tray spacing	0.45	m
fld	Flooding	85	%
$\alpha = \frac{A_d}{A_c} \bullet 100$	Downcomer area (A_d) as a percentage of total column cross-sectional area (A_c)	10	%

Calculations:

Formula/Source	**Description**	**Value for top**	**Value for bottom**	**Unit**

		section	section	
$F_{LV} = \frac{L_m}{V_m} \bullet \sqrt{\frac{\rho_V}{\rho_L}}$	Liquid-vapor flow factor	0.051	0.1006	-
K_1	constant from Fig. 11.27, C&R	8.1e-2	7.4e-2	-
$K_{1,corrected} = K_1 \bullet \left(\frac{\sigma}{0.02}\right)^{0.2}$	constant corrected for surface tension	7.44e-2	6.70e-2	-
$u_f = K_{1,corrected} \bullet \sqrt{\frac{\rho_L - \rho_V}{\rho_v}}$	flooding vapor velocity	0.960	0.814	m/s
$u_v = u_f \bullet \frac{fld}{100}$	maximum vapor velocity @ flooding estimate	0.816	0.692	m/s
$\Phi_{v,\max} = \frac{Vm \bullet MW_V}{\rho_V \bullet 3600}$	maximum volumetric vapor flow rate	6.684	3.604	m^3/s
$A_n = \frac{\Phi_{v,\max}}{u_v}$	net area available for V/L disengagement, normally equal to Ac-Ad, for a single pass plate	8.186	5.206	m^2
$A_c = \frac{A_n}{(1 - \frac{\alpha}{100})}$	Total cross-sectional area of the column	9.096	5.785	m^2
$D_c = \sqrt{\frac{4 \bullet A_c}{\pi}}$	Column diameter	3.403	2.714	m
D_c	Set Column diameter at largest	3.403		m

Liquid flow pattern

Formula/Source	**Description**	**Value for top section**	**Value for bottom section**	**Unit**
$\Phi_{L,\max} = \frac{Lm \bullet MW_L}{\rho_L \bullet 3600}$	maximum volumetric liquid flow rate	0.0270	0.0298	m^3/s
	Check liquid flow pattern in Fig. 11.28	single pass plate	single pass plate	-

Provisional Plate Design

Initial estimates

Formula/Source	**Description**	**Value**	**Unit**
D_c	Column diameter	3.424	m
$A_c = \frac{1}{4} \bullet \pi \bullet D_c^{\ 2}$	Total cross-sectional area of the column	9.210	m^2
$A_d = \frac{\alpha}{100} \bullet A_c$	Cross-sectional area of downcomer	0.921	m^2
$A_n = A_c - A_d$	net area available for V/L disengagement, normally equal to Ac-Ad, for a single pass plate	8.289	m^2
$A_a = A_c - 2 * A_d$	active, or bubbling area, equal to Ac-2Ad for	7.368	m^2

	single pass plates		
$\beta = \frac{A_h}{A_a} \bullet 100$	Ah as % of Aa. Ah is the total hole area, the total area of all holes	10	%
$A_h = \frac{\beta}{100} \bullet A_a$	Total area of holes	0.737	m^2
l_w	Weir length (Fig. 11.31)	3.204	m
$h_w \quad (or\, h_o)$	Weir height (take hw=ho)	50	mm
D_h	Hole diameter	5	mm
γ	Take plate thickness	5	mm

Weeping

Formula/Source	Description	Value for top section	Unit
$\Phi_{L,\max} = \frac{L_m \bullet MW_L}{3600}$	maximum liquid rate	14.954	kg/s
$\Phi_{L,\min} = \Phi_{L,\max} \bullet 0.70$	minimum liquid rate @ 70% turn-down	10.468	kg/s
$h_{ow,\max} = 750 \bullet \left(\frac{\Phi_{L,\max}}{\rho_L \bullet l_w} \right)^{\frac{2}{3}}$	maximum height of liquid crest over downcomer weir	37	mm liquid
$h_{ow,\min} = 750 \bullet \left(\frac{\Phi_{L,\min}}{\rho_L \bullet l_w} \right)^{\frac{2}{3}}$	minimum height of liquid crest over downcomer weir	29	mm liquid
$(h_o + h_{ow,\min})$		79	mm liquid
K_2	constant from C&R, fig. 11.30	30.7	-
$u_{h,\min} = \frac{K_2 - 0.9 \bullet (25.4 - D_h)}{\sqrt{\rho_V}}$	minimum vapor velocity through holes	4.316	m/s
$u_{h,\min,act} = \frac{\Phi_{V,\max} \bullet 0.70}{A_h}$	actual minimum vapor velocity through holes	6.429	m/s
$u_{h,\min,act} > u_{h,\min}$		OK	

Plate pressure drop

Formula/Source	Description	Value	Unit
$u_{h,\max} = \frac{\Phi_{V,\max}}{A_h}$	maximum vapor velocity through holes	9.185	m/s

$\delta = \frac{\gamma}{D_h}$	plate thickness/hole diameter	1.0	-
$\frac{A_h}{A_p}$	(= Ah/Aa, assumption)	0.1	-
C_0	Orifice coefficient (from Fig. 11.34)	0.84	-
$h_d = 51 \bullet \left(\frac{u_{h,\max}}{C_0}\right)^2 \bullet \left(\frac{\rho_V}{\rho_L}\right)$	dry plate pressure drop	36	mm liquid
$h_r = \frac{12500}{\rho_L}$	residual head	23	mm liquid
$h_t = h_d + (h_w + h_{ow}) + h_r$	total plate drop	138	mm liquid
$\Delta P_{tot,plate} = 9.81 \bullet h_t \bullet 0.001 \bullet \rho_L$	pressure difference plate	751	Pa

Downcomer liquid back-up

Formula/Source	Description	Value	Unit
$h_{ap} = h_w - 5$	height of the bottom edge of the apron above the plate	45	mm
$h_{dc} = 166 \bullet \left(\frac{L_m \bullet MW_L}{\rho_L \bullet A_m \bullet 3600}\right)^2$	head loss in downcomer	9.96	mm
$h_b = (h_w + h_{ow}) + h_t + h_{dc}$	height of liquid backed up in downcomer	228	mm
Am=Aap	Area term in eq. 11.92. Aap or Ad? Use whichever is smaller	0.110	m^2
$A_{ap} = h_{ap} \bullet 0.001 \bullet l_w$	Clearance area under the downcomer	0.110	m^2
$0.5 \bullet (t_s + h_w \bullet 0.001)$	froth height=0.5*(plate spacing+weir height)	0.25	m
$h_b < 0.5 \bullet (t_s + h_w \bullet 0.001)$	Check hb<0.5*(plate spacing+weir height)	OK	-

Downcomer Residence Time

Formula/Source	Description	Value	Unit
$t_r = \frac{A_d \bullet h_b \bullet \rho_L}{L_m \bullet MW_L} * 3600$	residence time	7.7	s
tr>3		OK	-

Check Entrainment

Formula/Source	Description	Value	Unit
$u_{v,act} = \frac{\Phi_{V,\max}}{A_n}$	actual velocity, based on net area	0.816	m/s

$percent\ flooding = \frac{u_{V,act}}{u_f} \cdot 100$		85	%
Ψ	frac entrainment phi (Fig. 11.29)	0.09	-
Entrainment OK?		OK	-

Perforated Area

Formula/Source	Description	Value	Unit
lw/Dc		0.72	-
Θ_C	from Fig. 11.32	99	deg
$\Theta_D = 180 - \Theta_C$	angle subtended at plate edge by unperforated srips	81	deg
Wcz	width of calming zones	100	mm
Wues	width of support ring for sectional plates	50	mm
$ml_{ues} = \left(D_c - W_{ues} \cdot 0.001\right) \cdot \pi \cdot \frac{\Theta_D}{180}$	mean length unperforated edge strips	4.74	m
Aues=Wues*mlues	area of unperforated edge strips	0.237	m^2
$A_{cz} = 2 \cdot W_{cz} \cdot 0.001 \cdot \left(l_w \cdot 0.001 - 2 \cdot W_{cz} \cdot 0.001\right)$	area of calming zones	0.45	m^2
$A_p = A_a - \left(A_{ues} + A_{cz}\right)$	perforated area	6.59	m^2
$\frac{l_p}{D_h} = \sqrt{\frac{0.9 \cdot A_p}{A_h}}$	hole pitch	2.85	-
Hole pitch within satisfactory limits? (2.5-4.0)	From Fig 11.33	OK	-

Number of holes

Formula/Source	Description	Value	Unit
$N = \frac{A_h}{\frac{1}{4} \cdot \pi \cdot {D_h}^2}$	Number of Holes	37060	-

APPENDIX 13: MODEL FOR THE HYDROISOMERIZATION OF HEPTANE

By assuming the PCP (protonated cyclopropane) mechanism for hydroisomerization, the following reactions are mechanistically possible:

1) n-C7 ↔ 2-MHx
2) n-C7 ↔ 3-MHx
3) 2-MHx ↔ 3-MHx
4) 2-MHx ↔ 2,2-DMP
5) 2-MHx ↔ 2,3-DMP
6) 2-MHx ↔ 2,4-DMP
7) 3-MHx ↔ 2,3-DMP
8) 3-MHx ↔ 3,3-DMP
9) 3-MHx ↔ 3-EP
10) 2,2-DMP ↔ 2,3-DMP
11) 2,3-DMP ↔ 2,4-DMP
12) 2,3-DMP ↔ 3,3-DMP
13) 2,4-DMP ↔ 2,2,3-TMB

For each of these reactions a kinetic equation can be derived. In general, for reaction (i) A↔B this equation holds:

$$r_i = k_i[A] - \frac{k_i}{K_i}[B]$$

By applying the above stated reaction network, the following rate equations can be derived for the isomerization reactions:

$$\frac{d[nC7]}{d\tau} = -r_1 - r_2 - r_C$$

what is r_c?

$$\frac{d[2MHx]}{d\tau} = r_1 - r_3 - r_4 - r_5 - r_6 - r_C$$

$$\frac{d[3MHx]}{d\tau} = r_2 + r_3 - r_7 - r_8 - r_9 - r_C$$

$$\frac{d[22DMP]}{d\tau} = r_4 - r_{10} - r_C$$

$$\frac{d[23DMP]}{d\tau} = r_5 + r_7 + r_{10} - r_{11} - r_{12} - r_C$$

$$\frac{d[24DMP]}{d\tau} = r_6 + r_{11} - r_{13} - r_C$$

$$\frac{d[33DMP]}{d\tau} = r_8 + r_{12} - r_C$$

$$\frac{d[3EP]}{d\tau} = r_9 - r_C$$

$$\frac{d[223TMB]}{d\tau} = r_{13} - r_C$$

The average reaction rates (of both forward and backward reaction) and their corresponding rate constants were classified into the three categories based on the observed kinetic data, all reactions in each category were assumed to have equal rate constants, so in fact only three rate constants had to be determined,:

Catalyst I:	Fast reactions:	1, 2, 3, 5, 6, 11 and 12
	Intermediate:	4, 7, 10 and 13
	Slow reactions:	8 and 9
Catalyst II:	Fast reactions:	8, 9, 11, 12 and 13
	Intermediate:	1, 3 and 6
	Slow reactions:	2, 4, 5 and 10

Furthermore, all C7 isomers have a certain tendency to crack. In this reaction the molecule reacts with hydrogen to form propane and isobutane. The rate of cracking for some component A is given by:

$$r_C = k_C[A]\underset{1}{\cdot}[H_2]^{p.} \qquad p = 0\ ?$$

These reactions are assumed to be first order in reactant, zero order in hydrogen and irreversible. The cracking coefficient k_C is assumed to be only a function of the degree of branching, so four rate constants had to be determined:

$$k_{C,linear} < k_{C,monobranched} < k_{C,\ dibranched} < k_{C,\ tribranched}$$

For catalyst I (Pt/HBEA) this model was fitted to the experimental results from Chao et al. For catalyst II (Ni/SiO2) data from Emett was used. The equilibrium constants were calculated using ASPEN and the relative rate constants were calculated using a gas phase plug flow model in Excel.

The actual weight based rate constants (k_W in $m^3s^{-1}kg^{-1}$) were calculated using the given experimental conditions and the total conversion using the following equations for an *irreversible* first order reaction in a PFR. The validity of this equation is limited as in reality the reacting mixture is approaching equilibrium.

$$k_V\tau = \frac{W}{V}k_W\tau = \ln\left(\frac{1}{1-X}\right)$$

$$WHSV_A = \frac{3600\cdot C_{A0}}{W}\phi_V = \frac{3600\cdot C_{A0}}{W}\cdot\frac{V}{\tau}$$

Hence,

$$k_W = \frac{WHSV_A}{3600\cdot C_{A0}}\ln\left(\frac{1}{1-X}\right)$$

In case of an ideal gas:

$$C_{A0} = \frac{n_{A0}M_A}{V} = \frac{p_{A0}M_A}{RT} = \frac{n_{A0}}{n_0}\cdot\frac{pM_A}{RT}$$

For the volumetric rate constants we need the catalyst bed density, which is assumed to be 1000 kg/m^3.

$$k_v = \frac{W}{V} k_W = 1000 k_w$$

The following rate constants were found at the experimental conditions:

Reaction number	Cat I 210°C k_V (s^{-1})	Cat II 313°C k_V (s^{-1})
r1	0.0975	0.00229
r2	0.0925	6.5E-06
r3	0.0643	0.00180
r4	0.0229	2.9E-06
r5	0.0419	3.1E-06
r6	0.0383	0.00084
r7	0.0204	3.2E-06
r8	0.0029	0.00478
r9	0.0017	0.00220
r10	0.0254	5.5E-06
r11	0.0656	0.01085
r12	0.0528	0.00880
r13	0.0121	0.00743

Table 1: Rate constants for isomerization

reactant	cat I 210°C k_C (s^{-1})	cat II 313°C k_C (s^{-1})
n-C7	0.0066	0
2-MHx	0.0090	0.00039
3-MHx	0.0090	0.00039
3-EP	0.0090	0.00039
2,2-DMP	0.0212	0.00039
2,3-DMP	0.0212	0.00039
2,4-DMP	0.0212	0.00039
3,3-DMP	0.0212	0.00039
2,2,3-TMB	0.0480	0.00039

Table 2: Rate constants for cracking

The temperature dependency of these rate constants was established by applying the Arrhenius equation to the data. For the isomerization reactions, all *average* reaction rates were assumed to have equal activation energies, being 137.5 kJ/mol. The equilibrium shift by temperature change was implemented by attributing different activation energies to the forward and backward reaction respectively.

	Cat I k°_{V1} s^{-1}	k°_{V-1} s^{-1}	E_{A1} kJ/mol	E_{A-1} kJ/mol	Cat II k°_{V1} s^{-1}	k°_{V-1} s^{-1}	E_{A1} kJ/mol	E_{A-1} kJ/mol
r1	4.33E+13	9.64E+13	135.5	142.1	2.66E+09	6.53E+09	135.5	142.2
r2	5.29E+13	6.46E+13	136.3	139.8	8.89E+06	1.09E+07	136.3	139.8
r3	7.14E+13	3.92E+13	139.3	136.0	4.84E+09	2.40E+09	139.3	136.0
r4	3.56E+12	7.14E+13	131.2	141.4	1.47E+06	2.95E+07	131.2	141.5
r5	3.21E+13	7.14E+13	137.7	137.4	5.96E+06	1.33E+07	137.7	137.4
r6	1.07E+13	1.07E+14	133.6	139.1	6.55E+08	7.22E+09	133.5	139.1
r7	9.67E+12	3.92E+13	135.6	138.5	3.99E+06	1.62E+07	135.6	138.5
r8	5.32E+11	1.07E+13	131.7	139.4	2.66E+09	5.90E+10	131.7	139.4
r9	7.96E+10	1.31E+13	126.6	139.4	4.39E+08	6.52E+10	126.6	139.4
r10	8.73E+13	8.75E+12	143.7	133.1	3.60E+07	3.61E+06	143.7	133.2
r11	2.38E+13	1.07E+14	134.5	140.3	1.08E+10	4.83E+10	134.5	140.3
r12	1.95E+13	9.64E+13	134.6	139.3	8.82E+09	4.83E+10	134.6	139.3
r13	7.14E+13	2.15E+13	146.1	135.4	7.96E+10	2.17E+10	146.1	135.4

Table 3: Arrhenius parameters and activation energies for isomerization

For the cracking reactions, the activation energy was determined from experimental data at different temperatures. It was found to be 175 kJ/mol and assumed to be equal for all cracking species.

reactant	cat I k (1/s)	cat II k (1/s)
n-C7	5.59E+16	0
2-MHx	7.56E+16	1.56E+12
3-MHx	7.56E+16	1.56E+12
3-EP	7.56E+16	1.56E+12
2,2-DMP	1.79E+17	1.56E+12
2,3-DMP	1.79E+17	1.56E+12
2,4-DMP	1.79E+17	1.56E+12
3,3-DMP	1.79E+17	1.56E+12
2,2,3-TMB	4.05E+17	1.56E+12

Table 4: Arrhenius parameters and activation energies for cracking

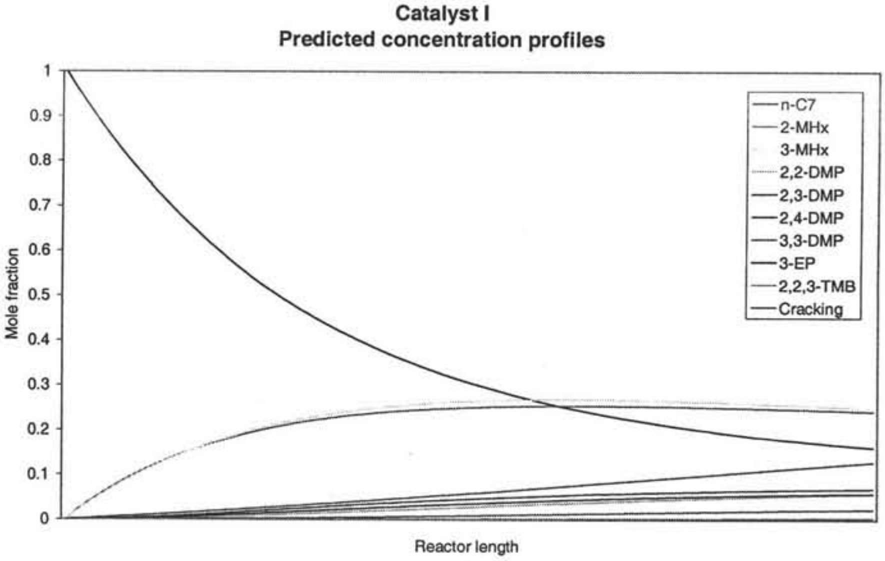
To evaluate the goodness-of-fit the relative deviations of the model and the experimental data were calculated:

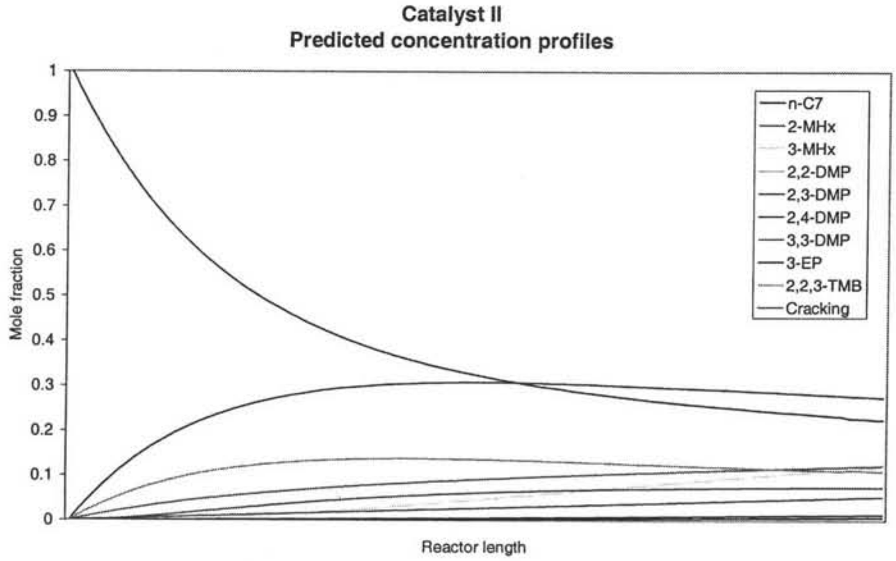
Product	Relative error from exp. data (%)	
	cat I	cat II
n-C7	0.2	28.2
2-MHx	3.1	8.5
3-MHx	3.2	0.1
3-EP	1.5	20.9
2,2-DMP	5.1	20.9
2,3-DMP	8.0	9.8
2,4-DMP	12.0	9.2
3,3-DMP	12.4	10.4
2,2,3-TMB	0.9	15.5
Cracking products	0.1	2.0

Table 5: Goodness-of-fit analysis

It is clear that the especially in the case of catalyst II the error is quite large. Therefore the predictive abilities of the model are poor.

In the following figures the fitted concentration profiles under experimental conditions are shown for catalyst I and II.





List of symbols:

r_i	Reaction rate of component i (mol/m^{3}s)
r_C	Reaction rate of cracking (mol/m^{3}s)
k_i	First order reaction rate constant of component i (1/s)
k_C	First order reaction rate constant of cracking (1/s)
$[A]$	Concentration of component A (mol/m^3)
V	Catalyst bed volume (m^3)
W	Catalyst bed weight (kg)
X	Conversion (-)
τ	Residence time (s)
$WHSV_A$	Weight hourly space velocity of component A (1/h)
C_{A0}	Initial concentration of component A
ϕ_V	Volumetric feed flowrate (m^3/s)
n_{A0}	Number of moles of component A at inlet conditions (mol)
n_0	Total number of moles at inlet conditions (mol)
M_A	Molar mass of component A (kg/mol)
p_{A0}	Partial pressure of component A at inlet (Pa)
R	Gas constant (J/mol·K)
T	Temperature (K)
p	Pressure (Pa)

References:

Chao, K.-J.; Wu, H.-C.; Leu, L.-J.; Appl. Catal. A: Gen. 143, 1996, 223-243

Emett, P.H. (ed), Catalysis VI, Hydrocarbon Catalysis, London, Reinhold Pub. Corp., 1958, 542-567

APPENDIX 14: HEAT EXCHANGER SIZING CALCULATIONS

The heat exchanging design procedure is described in chapter 8. In this Appendix only the design calculations of heat exchanger E10 are demonstrated as an example. The only major difference between the design calculations of all heat exchangers is the estimation of the shell-side and tube-side coefficient and temperatures. If there is a phase change and there are two phases present, the correlations used are different than if there is no phase change (and only one phase present). If there is only one temperature on either the shell or tube side (e.g. condensation or vaporization), then the logarithmic temperature difference will be simplified. Detailed description can be found in Coulson & Richardson's Chemical Engineering Volume 6.

E10 Heat exchanger

1. Known variables and physical data from Aspen Plus:

Property	Description	Value	Unit
T1	inlet shell-side fluid temperature (C7 mix)	360.0	K
T2	outlet shell-side fluid temperature (C7 mix)	458.0	K
t1	inlet tube-side temperature (40 bar HP steam)	683.0	K
t2	outlet tube-side temperature (40 bar condensed steam)	523.3	K
Q	Net heat duty required	-3781.7	kW
$\Phi_{m,C7}$	Mass flow rate of liquid to be heated (C7)	1176.1	t/d
ΔH_{cond}	condensation enthalpy HP steam (@523.3 K)	1712.6	kJ/kg
$\rho_{C7,vapor}$	average density C7 vapor	3.30	kg/m3
μ_{C7}	Viscosity C7 stream	1.37e-5	Pas
$k_{f,C7}$	Thermal conductivity C7 stream	0.17	W/m K
Cp_{C7}	Average specific heat C7 stream	2.883	kJ/kg K
$\rho_{steam,V}$	density steam @ 683K	13.2	kg/m^3
$\rho_{condensed\ steam,L}$	density condensed steam @ 523K	568	kg/m^3
$k_{steam,L}$	Thermal conductivity condensed steam	0.62	W/m K
μ_{steamL}	Viscosity condensed steam	0.000198	Pas
Cp_{steamL}	Specific heat HP steam vapor	2.331	kJ/kg K
Cp_{steamV}	Specific heat HP steam liquid	4.87	kJ/kg K

2. Tube geometry:

Formula/Symbol	Description	Value	Unit
od	outside diameter	20.0	mm
id	inside diameter	16.8	mm
L	length	2.44	m
Atube=3.1416*od*0.001*L	area one tube	0.153	m^2

3. Area and number of tubes:

Formula/Source	**Description**	**Value**	**Unit**
$\Phi_{steam} = \frac{Q}{(t_1 - t_{cond,steam}) \cdot Cp + \Delta H_{cond,steam}}$	mass flow steam necessary	168.3	t/d
U_{guess}	Assumed overall heat transfer coefficient	950	$W/m^2\ K$
F_t	Choose one pass, one shell exchanger. [24] Fig 12.19	1.00	-
$\Delta T_{lm} = \frac{(T1\text{-}t2)\text{-}(T2\text{-}t1)}{\ln \frac{T1\text{-}t2}{T2\text{-}t1}}$	logarithmic mean temperature difference [24] eq. 12.4,	192.5	K
$\Delta T_m = F_t \cdot \Delta T_{lm}$	mean temperature difference	192.5	K
$A_{required} = \frac{Q \cdot 1000}{U_{guess} \cdot \Delta T_m}$	Required exchange area	23.1	m^2
$N_t = \frac{A_{required}}{A_{tube}}$	Total number of tubes	151	-

4. Tube arrangements

Formula/Source	**Description**	**Value**	**Unit**
Triangular or square pitch?	Choose triangular pitch		-
$P_t = 1.25 \cdot od$	pitch	25	mm
K_1	constant from [24] Table 12.4	0.319	-
n_1	constant from [24] Table 12.4	2.142	-
$D_b = od \cdot \left(\frac{Nt}{K1}\right)^{\frac{1}{n_1}}$	bundle diameter, [24] eq 12.3b	354	mm
Ncr=Db/Pt	number of tubes in center row	14	-

5. Shell-side coefficient (to be heated C7 vapor, Kern's method, single (phase)

Formula/Source	**Description**	**Value**	**Unit**
$\alpha = D_s - D_b$	Shell to bundle clearance Choose from Fig 12.10	60	mm
Ds=Db+alfa $D_s = D_b + \alpha$	inside shell diameter	414	mm
l_b	baffle spacing, usually equal to Ds	414	mm
$N_b = \frac{L}{l_b \cdot 0.001}$	number of baffles	5.89	-
N_{bact}	Actual number of baffles	6	-
$l_{b,act} = \frac{L}{N_{b,act}}$	Actual baffle spacing	407	mm

$A_s=\frac{(P_t\text{-od})\bullet 0.001}{Pt\bullet 0.001}\bullet Ds\bullet 0.001\bullet l_{b,act}\bullet 0.001$	area for cross flow	0.034	m^2
$v_{Shell}=\frac{\frac{\Phi_m\bullet 1000}{24\bullet 3600}}{\rho_{C7}\bullet A_s}$	shell velocity	122.35	m/s
$G_s=\frac{\frac{\Phi_m\bullet 1000}{24\bullet 3600}}{A_s}$	mass velocity	403.77	$kg/s/m^2$
$d_e=\left(\frac{1.10}{od}\right)\bullet\left(P_t^2\text{-}0.917\bullet od^2\right)$	shell equivalent diameter (ONLY VALID FOR TRIANGULAR PITCH!)	14	mm
$Re=\frac{G_s\bullet d_e\bullet 0.001}{\mu_{C7}}$	Reynolds number	420002	-
$Re=\frac{\rho_{C7}\bullet v_{Shell}\bullet d_e\bullet 0.001}{\mu_{C7}}$	Reynolds number	420002	-
$Pr=\frac{Cp\bullet 1000\bullet \mu_{C7}}{k_{f,C7}}$	Prandtl	0.33	
j_h	heat tranfser factor value from [24] figure 12.29	0.0010	-
$hs=\frac{kf}{de*0.001}\bullet jh\bullet Re\bullet Pr^{(1/3)}\bullet\left(\frac{\mu}{\mu_W}\right)^{0.14}$	neglect mu/muW	3438	W/m^2 K
L/Ds	tube length over shell diameter	5.9	
L/Ds	L/D should in 5-10 range OK?	OK	

6. Tube-side coefficient (steam condensing, 2 phase)

Formula/Source	**Description**	**Value**	**Unit**
$Pr_c=\frac{Cp_{steam,L}\bullet 1000\bullet \mu_{steam,L}}{k_{steam,L}}$	Prandtl number for condensate film	1.55	
$Wc=\Phi_{m,steam}$	Total condensate flow	1.95	kg/s
$\Gamma_V=\frac{W_c}{Nt\bullet\pi\bullet id\bullet 0.001}$	tube lading, condensate flow per unit length of tube	0.245	kg/m s
$v_{fluid}=\frac{\Phi_{steam}}{\rho_{steamL}\bullet A_{cross}}$	fluid velocity total condensation	0.103	m/s
$A_{cross}=\frac{1}{4}\bullet\pi\bullet(id\bullet 0.001)^2\bullet N_t$		0.033	m^2
$Re=\frac{\rho_{steamL}\bullet v_{fluid}\bullet id\bullet 0.001}{\mu_{steamL}}$	Reynolds number	4954	-
$Re_c=\frac{4\bullet\Gamma_V}{\mu_{SteamL}}$	Reynolds number	4954	-
β	constant from Fig 12.43 C&R	0.16	

$h_c=\beta \cdot k_{steamL} \cdot \left(\frac{\mu_{SteamL}{}^{2}}{\rho_L \cdot (\rho_L-\rho_V) \cdot 9.81}\right)^{-\frac{1}{3}}$	heat transfer constant tube side	4258	W/m^2 K
$h_i'=0.021 \cdot \frac{k_{steamL}}{id \cdot 0.001} \cdot Re^{0.8} \cdot Pr^{0.43}$		846	W/m^2 K
$h_{cBK}=h_i' \cdot \frac{1+\sqrt{\frac{\rho_{SteamL}}{\rho_{SteamV}}}}{2}$	tube side heat transfer coefficient	3198	W/m^2 K
Use hc or hcBLK?	whichever is higher	4258	W/m^2 K

7. Overall coefficient

Formula/Source	**Description**	**Value**	**Unit**
FC7	Fouling C7	5000	W/m^2 K
FH2O	Fouling water	6000	W/m^2 K
kw		50	W/m^2 K
hs	shell side heat transfer coefficient	3438	W/m^2 K
ht	tube side heat transfer coefficient	4258	W/m^2 K
$\frac{1}{U}=\frac{1}{h_s}+\frac{1}{FC7}+\frac{od \cdot 0.001 \cdot \ln\frac{od}{id}}{2 \cdot k_w}+\frac{od}{id} \cdot \frac{1}{FH2O}+\frac{od}{id} \cdot \frac{1}{h_t}$	inverse overall coefficient	0.00100	m^2 K/W
U	overall coefficient	996	W/m^2 K
OK with first estimate? If so, design is OK. If not, go to first estimate of U (section 3) again			

In this case the first estimate of the overall heat transfer coefficient U of 850 W/m^2 K was a little too low. With a trial-and-error method it is calculated that the overall heat transfer is 1016 W/m^2 K.

APPENDIX 15: CALCULATIONS FOR FURNACE

Area:

Property	Description	Value	Unit
ΔH_{gas}	enthalpy difference in gas that needs to be heated	6241.6	kW
q_r	radiant heat flux	30	kW/m^2
$A_{tubes} = \frac{\Delta H_{gas}}{q_r}$	total area of tubes	208.1	m^2

Number of tubes:

Property	Description	Value	Unit
$\Phi_{m,gas}$	mass flow gas to be heated	1032.7	t/d
$\rho_{gas,in}$	density gas to be heated, furnace in	5.48	kg/m^3
$\rho_{gas,in}$	density gas to be heated, furnace out	4.52	kg/m^3
$\rho_{gas} = \frac{\rho_{gas,in} + \rho_{gas,uit}}{2}$	average density gas to be heated	5.00	kg/m^3
$\Phi_{v,gas} = \frac{\left(\frac{\Phi_{m,gas} \cdot 1000}{24 \cdot 3600}\right)}{\rho_{gas}}$	volumetric flow rate of gas to be heated	2.39	m^3/s
D_t	diameter one tube	150	mm
$A_{cross,tube} = 0.25 \cdot \pi \cdot (D_t \cdot 0.001)^2$	cross-sectional area of one tube	0.0177	m^2
v_{gas}	velocity of gas to be heated	1.5	m/s
$N_t = \frac{\Phi_{v,gas}}{A_{cross,tube} \cdot v_{gas}}$	total number of tubes	91	-

Amount of fuel:

Property	Description	Value	Unit
$\Delta H_{combustion}$	heat of combustion	45200	kJ/kg
$\Phi_{m,fuel} = \frac{\Delta H_{gas}}{0.85 \cdot \Delta H_{combustion}}$	amount of fuel necessary	0.162	kg/s
$\Phi_{m,fuel}$	mass flow rate of fuel necessary	14.0	t/d

APPENDIX 16: EQUIPMENT SUMMARY

PUMPS, BLOWERS & COMPRESSORS – SUMMARY

EQUIPMENT NR.: **NAME :**	**P-01** **Reflux C-01**	**P-02** **Reflux C-02**	**P-03** **Bottoms C-02**	**P-04** **Reflux C-03**	**P-05** **Distillate C-03**
Type :	Centrifugal	Centrifugal	Centrifugal	Centrifugal	Centrifugal
Number :	2	2	2	2	2
Medium transferred :	<07>/<08>	<16>/<17>	<19>/<20>	<26>/<27>	<25>/<28>
Capacity					
[kg/s] :	17.740	100.296	32.066	77.841	13.612
[m^3/s] :	0.032	0.176	0.058	0.162	0.024
Density [kg/m^3] :	553	571	549	480	563.5
Pressure [bara] Suct. / Disch. :	1.0/1.0	1.0/1.0	1.4/1.4	1.0/1.0	1.0/10.0
Temperature In / Out [K] :	359/359	318/318	374/374	359/359	359/360
Power					
- Theor. :	4	39	10	29	22
- Actual :	6	52	13	39	32
Number					
- Theor. :					
- Actual :	2 (1)	2 (1)	2 (1)	2 (1)	2 (1)
Special Materials of Construction :					
Other :					

Remarks:

(1) One installed spare included.

Designers : M.A. Rijkse E.S.E.D van Kints V. Tjon Soei Len B.Vogelaar	Project ID-Number : **CPD3259** Date : June 19th 2001

PUMPS, BLOWERS & COMPRESSORS – SUMMARY

EQUIPMENT NR. : **NAME :**	**P-06** **Bottoms C-03**	**K-01** **Overhead C-01**	**K-02** **H_2 compressor R-01**	**K-03** **Feed R-02**
Type : **Number :**	Centrifugal 2			
Medium transferred :	<37>/<38>	<9>/<10>	<55>/<56>	<32>/<33>
Capacity **[kg/s] :** **[m^3/s] :**	 18.454 0.033	 7.486 2.266	 2.905 10.143	 11.952 21.267
Density [kg/m^3] :	555	3.303	0.286	0.562
Pressure [bara] **Suct. / Disch. :**	1.0/9.5	1.0/1.4	5.6/9.5	1.0/10.0
Temperature **In / Out [K] :**	367/367	359/367	504/609	422/585
Power [kW] **- Theor. :** **- Actual :**	 28 39	 101 112	 4426 4918	 6695 7440
Number **- Theor. :** **- Actual :**	 2 (1)			
Special Materials of Construction :				
Other :				

Remarks:

(1) One installed spare included.

Designers : M.A. Rijkse V. Tjon Soei Len	E.S.E.D van Kints B.Vogelaar	Project ID-Number : Date :	**CPD3259** June 19th 2001

COLUMNS & VESSELS - SUMMARY

EQUIPMENT NR. : **NAME :**	**C01** **Tailing Column**	**C02** **Topping Column**	**C03** **Reactant Sep. Column**	**V01** **C01 Reflux Accumulator**	**V02** **C02 Reflux Accumulator**
	Tray Column	Tray Column	Tray Column	Horizontal	Horizontal
Pressure [bara] :	1.25 / 1.0	1.38 / 1.0	1.04 / 1.0	1.0	1.0
Temp. [K] :	**397.5 / 362.0**	**372.7 / 336.7**	**366.4 / 359.9**	358.6	318.3
Volume [m^3] :				19.2 *(1)*	110.4 *(2)*
Diameter [m] :	3.57	5.34	5.05	1.80	3.30
L or H [m] :	21.15	35.2	34.0	7.30	13.10
Internals					
- Tray Type :	Sieve Trays	Sieve Trays	Sieve Trays	n.a.	n.a.
- Tray Number :	48	33	35	n.a.	n.a.
- Fixed Packing					
Type :	n.a.	n.a.	n.a.	n.a.	n.a.
Shape :	n.a.	n.a.	n.a.	n.a.	n.a.
- Catalyst					
Type :	n.a.	n.a.	n.a.	n.a.	n.a.
Shape :	n.a.	n.a.	n.a.	n.a.	n.a.
-					
-					
-					
Number					
-					
- Parallel :					
Materials of Construction *(2)* **:**	Trays: SS314 Column: CS	Trays: SS314 Column: CS	Trays: SS314 Column: CS	CS	CS
Other :					

Remarks:

(1) V01= effective volume = 9.6 m^3 for residence time of 5 minutes
(2) V02= effective volume = 55.2 m^3 for residence time of 5 minutes
(3) SS = Stainless Steel; CS = Carbon Steel

Designers :	E. van Kints M. Rijkse V. Tjon B. Vogelaar	Project ID-Number : Date :	**CPD3259** June 19th 2001

COLUMNS & VESSELS - SUMMARY

EQUIPMENT NR. : **NAME :**	**V03** **C03 Reflux Accumulator**				
	Horizontal				
Pressure [bara] :	1.0				
Temp. [K] :	359.0				
Volume [m^3] : **Diameter [m] :** **L or H [m] :**	95.1 *(1)* 3.10 12.50				
Internals **- Tray Type :** **- Tray Number :** **- Fixed Packing** **Type :** **Shape :** **- Catalyst** **Type :** **Shape :** - - -	 n.a. n.a. n.a. n.a. n.a. n.a.				
Number **- Series :** **- Parallel :**					
Materials of Construction *(2)* **:**	CS				
Other :					

Remarks:

(1) V03: effective volume = 48.63 m^3 for residence time of 5 minutes

(2) SS = Stainless Steel; CS = Carbon Steel

Designers :	E. van Kints V. Tjon	M. Rijkse B. Vogelaar	Project ID-Number Date	: :	**CPD3259** June 19th 2001

HEAT EXCHANGERS & FURNACES – SUMMARY

EQUIPMENT NR. : **NAME :**	**E06** **C03** **Reboiler**	**E07** **R01** **Vaporizer**	**E08** **R01** **Intercooler**	**E09** **R01** **Intercooler**	**E10** **M01** **Exchanger**
	Thermosyphon				Shell & tube: floating head
Substance					
Tubes :	LP Steam	HP Steam	Cooling W.	Cooling W.	HP Steam
Shell :	C_7/C_8	C_7/C_8	C_6/C_7	C_6/C_7	C_6/C_7
Duty [kW] :	27,442.6	9,477.7	495	495	3,800.0
Heat Exchange area [m^2] :	449.0	54.9			23.1
Number					
Series :	-	-			-
Parallel :	-	-			-
Pressure [bara]					
Tubes :	1.04	40.0	1.0	1.0	40.0
- Shell :	3.0	9.5	10.0	10.0	10.0
Temperature In / Out [°C]					
Tubes :	366.3 / 366.7	683.0 / 523.3	471.0 / na	na / 473.0	683.0 / 523.3
Shell :	372.7 / 373.7	367.0 / 473.0	293.0 / 313.0	293.0 / 313.0	360.0 / 458.0
Special Materials of Construction *(2* **:**	Tubes : CS Shell : CS	Tubes : CS Shell : CS	Tubes : CS Shell : CS	Tubes : CS Shell : CS	Tubes : CS Shell : CS
Other :					

Remarks:

Designers : E. van Kints M. Rijkse V. Tjon B. Vogelaar	Project ID-Number : **CPD3259** Date : May 29th 2001

HEAT EXCHANGERS & FURNACES – SUMMARY

EQUIPMENT NR. : **NAME :**	**E10** **M01** **Exchanger**	**E11** **K02** **Exchanger**	**E12** **K03** **Exchanger**	**F01** **R02** **Furnace**	
	Shell & tube: floating head	Shell & tube: floating head	na *(1)*		
Substance **- Tubes :** **- Shell :**	HP Steam C_6/C_7	H_2 Cooling W.	H_2/C6/C_7 Cooling W.	$H_2/C_6/C_7$ Furnace:$C_3/C_4/C_6$	
Duty [kW] :	3,800.0	-4,557.6	-6,034.7 *(2)*	6242	
Heat Exchange area [m^2] :	23.1	127.7	68.9 *(3)*	208.1	
Number **- Series :** **- Parallel :**	- -	- -	- -		
Pressure [bara] **- Tubes :** **- Shell :**	40.0 10.0	5.6 1.0	10.0 *(4)* 1.0	10.0 1.0	
Temperature In / Out [°C] **- Tubes :** **- Shell :**	683.0 / 523.3 360.0 / 458.0	504.0 / 396.2 293.0 / 313.0	*(5)* 293.0 / 313.0	473/573 furnace	
Special Materials of Construction :	Tubes : CS Shell : CS	Tubes : CS Shell : CS	Tubes : CS Shell : CS	SS	
Other :					

Remarks:

(1) E12 is three separate heat exchangers
(2) Values for heat duty given is area for all three combined
(3) Values for exchange area given is area for all three combined
(4) Pressure varies from 1.0-10.0 bar
(5) compressor is intercooled 3 times where temperature goes from 473 to 422 K

Designers :	E. van Kints	M. Rijkse	Project ID-Number	:	**CPD3259**
	V. Tjon	B. Vogelaar	Date	:	May 29th 2001

REACTORS & MEMBRANES – SUMMARY

EQUIPMENT NR. : **NAME :**	**R01** **Reactor 1**	**R02** **Reactor 2**	**M01** **Membrane 1**	**M02** **Membrane 2**	
	Vertical	Vertical	Block	Block	
Pressure [bara] :	9.50 / 8.66	10.0 / 9.96	10.0 / 1.00	8.66 / 5.60	
Temp. [K] :	471 / 473	573 / 575	458 / 489	506 / 404	
Volume [m^3] :	151	194	50	4	
Diameter [m] :	3.7	4.2	4	2	
L or H [m] :	14	14	3	1	
Internals					
- Tray Type :	N/A	N/A	N/A	N/A	
- Tray Number :	N/A	N/A	N/A	N/A	
- Fixed Packing					
Type :	N/A	N/A	N/A	N/A	
Shape :	N/A	N/A	N/A	N/A	
- Catalyst					
Type :	Pt/Hβ	Ni/ASA	N/A	N/A	
Shape :	Spheres	Spheres	N/A	N/A	
- Membrane :	N/A	N/A	ZSM-5	Silica	
Number					
- Series :	1	1	1	1	
- Parallel :	-	-	-	-	
Materials of Construction *(1)* **:**	SS	SS	CS	SS	
Other :					

Remarks:
(1) SS = Stainless Steel; CS = Carbon Steel

Designers :	E.S.E.D. van Kints	M.A. Rijkse	Project ID-Number :	**CPD3259**
	V.F.M. Tjon-Soei-Len	B.M. Vogelaar	Date :	June 1st 2001

APPENDIX 17: EQUIPMENT SPECIFICATION SHEETS

CENTRIFUGAL PUMP – SPECIFICATION SHEET

EQUIPMENT NUMBER	:	**P-05**	**Operating**	:	1
NAME	:	**Distillate C03 pump**	**Installed Spare**	:	1

Service	:	Distillate pump
Type	:	Radial Multistage Centrifugal
Number	:	2

Operating Conditions & Physical Data

Pumped liquid			C7-isomers		
Temperature	(T)	**[K]**	359.0		
Density	(ρ)	**[kg/m^3]**	564		
Viscosity	(η)	**[N·s/m^2]**	0.0002		
Vapour Pressure	(p_v)	**[bara]**	0.97	**at Temperature [K]**	359.0

Power

Capacity	(Φ_v)	**[m^3/s]**	0.024	
Suction Pressure	(p_s)	**[bara]**	1.00	
Discharge Pressure	(p_d)	**[bara]**	10.00	
Theoretical Power		**[kW]**	22	$\{=\Phi_v \cdot (p_d - p_s) \cdot 10^2\}$
Pump Efficiency		**[-]**	0.68	
Power at Shaft		**[kW]**	32	

Construction Details *(1)*

RPM		1750	**Nominal diameter**		
Drive		Electrical	**Suction Nozzle**	**[...]**	
Type electrical motor			**Discharge Nozzle**	**[...]**	
Tension	**[V]**	380	**Cooled Bearings**		**Yes / No**
Rotational direction		**Clock /** ~~**Counter Cl.**~~	**Cooled Stuffing Box**		**Yes / No**
			Smothering Gland		**Yes / No**
Foundation Plate		**Combined /** ~~**two parts**~~	**If yes**		
			- Seal Liquid		**Yes / No**
Flexible Coupling		Yes	**- Splash Rings**		**Yes / No**
Pressure Gauge Suction		No	**- Packing Type**		
Pressure Gauge Discharge		Yes	**- Mechanical Seal**		**Yes / No**
Min. Overpressure above p_v/p_m	**[bar]**		**- N.P.S.H.** $\{=p_m \cdot \rho g\}$	**[m]**	

Construction Materials *(2)*

Pump House	MS	**Wear Rings**	
Pump Rotor	HT Steel	**Shaft Box**	
Shaft	HT Steel		
Special provisions	none		
Operating Pressure [bara]		**Test Pressure [bara]**	

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Designers : M.A. Rijkse	E.S.E.D van Kints	Project ID-Number	:	**CPD3259**
V. Tjon Soei Len	B.Vogelaar	Date	:	June 19th 2001

CENTRIFUGAL PUMP – SPECIFICATION SHEET

EQUIPMENT NUMBER : P-06	**Operating** : 1
NAME : Bottoms C03 pump	**Installed Spare** : 1

Service : Bottoms C03
Type : Rasial Multistage Centrifugal
Number : 2

Operating Conditions & Physical Data

Pumped liquid : C7-isomers
Temperature (T) **[K]** : 366.7
Density (ρ) **[kg/m^3]**: 555
Viscosity (η) **[N·s/m^2]** : 0.0002
Vapour Pressure (p_v) **[bara]** : 1.02 **at Temperature [°C]** :366.7

Power

Capacity (Φ_v) **[m^3/s]** : 0.033
Suction Pressure (p_s) **[bara]** : 1.04
Discharge Pressure (p_d) **[bara]** : 9.5
Theoretical Power **[kW]** : 28 $\{= \Phi_v \cdot (p_d - p_s) \cdot 10^2\}$
Pump Efficiency **[-]** : 0.72
Power at Shaft **[kW]** : 39

Construction Details *(1)*

RPM : 1750	**Nominal diameter**
Drive : Electrical	**Suction Nozzle** [...] :
Type electrical motor :	**Discharge Nozzle** [...] :
Tension [V] : 380	**Cooled Bearings** : **Yes / No**
Rotational direction : **Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box** : **Yes / No**
	Smothering Gland : **Yes / No**
Foundation Plate : **Combined / ~~two parts~~**	**If yes**
	- Seal Liquid : **Yes / No**
Flexible Coupling : Yes	**- Splash Rings** : **Yes / No**
Pressure Gauge Suction : No	**- Packing Type** :
Pressure Gauge Discharge : Yes	**- Mechanical Seal** : **Yes / No**
Min. Overpressure above	**- N.P.S.H.** **[m]**:
p_v/p_m **[bar]** :	$\{= p_m \cdot \rho g\}$

Construction Materials (2)

Pump House : MS	**Wear Rings** :
Pump Rotor : HT Steel	**Shaft Box** :
Shaft : HT Steel	
Special provisions :none	
Operating Pressure **[bara]** :	**Test Pressure** **[bara]** :

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Designers : M.A. Rijkse E.S.E.D van Kints V. Tjon Soei Len B.Vogelaar	Project ID-Number : **CPD3259** Date : June 19th 2001

CENTRIFUGAL COMPRESSOR – SPECIFICATION SHEET

EQUIPMENT NUMBER : **K-01** **Operating** : 1
NAME : **Overhead compressor C01** **Installed Spare** : 1

Service : Overhead compressor C01
Type : Centrifugal
Number : 2

Operating Conditions & Physical Data

Compressed gas : C6/C7 isomers
Temperature (T) **[K]** : 358.6
Density (ρ) **[kg/m^3]**: 3.30
Viscosity (η) **[N·s/m^2]** : 1.2 E –5
Vapour Pressure (p_v) **[bara]** : 1.00 **at Temperature [K]** : 358.6

Power

Capacity (Φ_v) **[m^3/s]** : 2.266
Suction Pressure (p_s) **[bara]** : 1.0
Discharge Pressure (p_d) **[bara]** : 1.4
Theoretical Power **[kW]** : 101 $\{= \Phi_v \cdot (p_d - p_s) \cdot 10^2\}$
Pump Efficiency **[-]** : 0.78
Power at Shaft **[kW]** : 112

Construction Details *(1)*

RPM	:	**Nominal diameter**	
Drive	: Electrical	**Suction Nozzle [...]**	:
Type electrical motor	:	**Discharge Nozzle [...]**	:
Tension [V]	: 380	**Cooled Bearings**	: **Yes / No**
Rotational direction	: **Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**	: **Yes / No**
		Smothering Gland	: **Yes / No**
Foundation Plate	: **Combined / ~~two parts~~**	**If yes**	
		- Seal Liquid	: **Yes / No**
Flexible Coupling	: Yes	**- Splash Rings**	: **Yes / No**
Pressure Gauge Suction	: No	**- Packing Type**	:
Pressure Gauge Discharge	: Yes	**- Mechanical Seal**	: **Yes / No**
Min. Overpressure above		**- N.P.S.H. [m]**	:
p_v/p_m **[bar]**	:	$\{= p_m \cdot \rho \cdot g\}$	

Construction Materials *(2)*

Pump House	: MS	**Wear Rings**	:
Pump Rotor	: HT Steel	**Shaft Box**	:
Shaft	: HT Steel		
Special provisions	:none		
Operating Pressure [bara]	:	**Test Pressure [bara]**	:

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Designers : M.A. Rijkse	E.S.E.D van Kints	Project ID-Number	: **CPD3259**
V. Tjon Soei Len	B.Vogelaar	Date	: June 19th 2001

CENTRIFUGAL COMPRESSOR – SPECIFICATION SHEET

EQUIPMENT NUMBER : **K-02**
NAME : **Hydrogen compressor R01**
Operating : 1
Installed Spare : 1

Service : Hydrogen Compressor
Type : Centrifugal
Number : 2

Operating Conditions & Physical Data

Compressed gas : Hydrogen
Temperature **(T)** **[K]** : 504.2
Density **(ρ)** **[kg/m^3]**: 0.269
Viscosity **(η)** **[N·s/m^2]** : 1.3 E -5
Vapour Pressure **(p_v)** **[bara]** : n.a. **at Temperature [K]** : 504.2

Power

Capacity **(Φ_v)** **[m^3/s]** : 10.811
Suction Pressure **(p_s)** **[bara]** : 5.6
Discharge Pressure **(p_d)** **[bara]** : 10.0
Theoretical Power **[kW]** : 4426 $\{= \Phi_v \cdot (p_d - p_s) \cdot 10^2\}$
Pump Efficiency **[-]** : 0.78
Power at Shaft **[kW]** : 7918

Construction Details *(1)*

RPM :
Drive : Electrical
Type electrical motor :
Tension **[V]** : 380
Rotational direction : **Clock /** **~~Counter Cl.~~**
Foundation Plate : **Combined /** **~~two parts~~**
Flexible Coupling : Yes
Pressure Gauge Suction : No
Pressure Gauge Discharge : Yes
Min. Overpressure above **p_v/p_m** **[bar]** :

Nominal diameter
Suction Nozzle **[…]** :
Discharge Nozzle **[…]** :
Cooled Bearings : **Yes / No**
Cooled Stuffing Box : **Yes / No**
Smothering Gland : **Yes / No**
If yes
- Seal Liquid : **Yes / No**
- Splash Rings : **Yes / No**
- Packing Type :
- Mechanical Seal : **Yes / No**
- N.P.S.H. **[m]**: $\{= p_m \cdot \rho g\}$

Construction Materials *(2)*

Pump House : MS
Pump Rotor : HT Steel
Shaft : HT Steel
Special provisions :none
Operating Pressure **[bara]** :

Wear Rings :
Shaft Box :
Test Pressure **[bara]** :

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Designers : M.A. Rijkse	E.S.E.D van Kints	Project ID-Number :	**CPD3259**
V. Tjon Soei Len	B.Vogelaar	Date :	June 19th 2001

CENTRIFUGAL COMPRESSOR – SPECIFICATION SHEET

EQUIPMENT NUMBER	: **K-03**	**Operating**	: 1
NAME	: **Feed compressor R02**	**Installed Spare**	: 1

Service : Feed compressor R02
Type : Centrifugal
Number : 2

Operating Conditions & Physical Data

Compressed gas			:	C7 isomers/hydrogen
Temperature	**(*T*)**	**[K]**	:	422.1
Density	**(ρ)**	**[kg/m^3]**	:	0.616
Viscosity	**(η)**	**[N·s/m^2]**	:	1.2 E -5
Vapour Pressure	**(p_v)**	**[bara]**	:	22.0 **at Temperature [K]** : 422.1

Power

Capacity	**(Φ_v)**	**[m^3/s]**	:	19.405	
Suction Pressure	**(p_s)**	**[bara]**	:	1.0	
Discharge Pressure	**(p_d)**	**[bara]**	:	10.0	
Theoretical Power		**[kW]**	:	6695	$\{ = \Phi_v \cdot (p_d - p_s) \cdot 10^2 \}$
Pump Efficiency		**[-]**	:	0.78	
Power at Shaft		**[kW]**	:	7440	

Construction Details *(1)*

RPM	:	**Nominal diameter**	
Drive	: Electrical	**Suction Nozzle [...]**	:
Type electrical motor	:	**Discharge Nozzle [...]**	:
Tension [V]	: 380	**Cooled Bearings**	: **Yes / No**
Rotational direction	: **Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**	: **Yes / No**
		Smothering Gland	: **Yes / No**
Foundation Plate	: **Combined / ~~two parts~~**	**If yes**	
		- Seal Liquid	: **Yes / No**
Flexible Coupling	: Yes	**- Splash Rings**	: **Yes / No**
Pressure Gauge Suction	: No	**- Packing Type**	:
Pressure Gauge Discharge	: Yes	**- Mechanical Seal**	: **Yes / No**
Min. Overpressure above		**- N.P.S.H. [m]**	:
p_v/p_m [bar]	:	$\{ = p_m \cdot \rho g \}$	

Construction Materials *(2)*

Pump House	: MS	**Wear Rings**	:
Pump Rotor	: HT Steel	**Shaft Box**	:
Shaft	: HT Steel		
Special provisions	:none		
Operating Pressure [bara]	:	**Test Pressure [bara]**	:

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Designers : M.A. Rijkse	E.S.E.D van Kints	Project ID-Number	: **CPD3259**
V. Tjon Soei Len	B.Vogelaar	Date	: June 19th 2001

DISTILLATION COLUMN – SPECIFICATION SHEET

EQUIPMENT NUMBER : C01
NAME : Tailing Column

General Data

Service : - distillation / ~~extraction~~ / ~~absorption~~ / ———
Column Type : - ~~packed~~ / tray / ~~spray~~ / ———
Tray Type : - ~~cap~~ / sieve / ~~valve~~ / ———
Tray Number *(1)*
- **Theoretical** : 25
- **Actual** : 48
- **Feed (actual)** : 21

Tray Distance (HETP) [m] : 0.450 **Tray Material** : **SS314** *(2)*
Column Diameter [m] : 3.570 **Column Material** : **CS** *(2)*
Column Height [m] : 21.150
Heating : - ~~none~~ / ~~open steam~~ / reboiler / ——— *(3)*

Process Conditions

Stream Details	Feed		Top		Bottom		Reflux / ~~Absorbent~~		~~Extractant~~ / ~~side stream~~	
Temp. [K]	: 373		: 362		: 398		: 359			
Pressure [bara]	: 1.25		: 1.0		: 1.25		: 1.0			
Density [kg/m³]	: 547.65		: 3.30		: 553.55		: 547.22			
Mass Flow [t/d]	: 907.2		: 2179.6		: 260.4		: 1532.72			
Composition	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**
Hydrogen	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
Propane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
Isobutane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
N-C6	0.164	0.142	0.219	0.200	0.000	0.000	0.135	0.120		
2-MP	0.072	0.062	0.096	0.088	0.000	0.000	0.047	0.042		
3-MP	0.067	0.058	0.089	0.081	0.000	0.000	0.048	0.042		
N-C7	0.212	0.213	0.280	0.297	0.006	0.005	0.406	0.419		
2-MHx	0.089	0.090	0.119	0.126	0.000	0.000	0.133	0.138		
3-MHx	0.115	0.116	0.154	0.163	0.000	0.000	0.182	0.188		
2,2-DMP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
2,3-DMP	0.032	0.032	0.043	0.045	0.000	0.000	0.048	0.049		
2,4-DMP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
3,3-DMP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
3-EP	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
2,2,3TMB	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000		
2-MHEPT	0.100	0.115	0.000	0.000	0.401	0.402	0.000	0.000		
3-MHEPT	0.079	0.091	0.000	0.000	0.317	0.317	0.000	0.000		
4-MHEPT	0.032	0.036	0.000	0.000	0.127	0.127	0.000	0.000		
2,3-DMHx	0.019	0.021	0.000	0.000	0.075	0.075	0.000	0.000		
2,4-DMHx	0.019	0.022	0.001	0.001	0.074	0.074	0.001	0.002		

Column Internals *(4)*

Trays *(5)*
Number of
~~caps~~ / sieve holes / ——— : **37060**
Active Tray Area [m²] : **7.368**
Weir Length [mm] : **2.598**

Packing *Not Applicable*
Type :
Material :
Volume [m³] :
Length [m] :
Width [m] :
Height [m] :

Remarks:
(1) Tray numbering from top to bottom.
(2) SS = Stainless Steel CS = Carbon Steel.
(3) Reboiler is E01: operates with LP steam
(4) Tray layout valid for whole column

Designers : E. van Kints M. Rijkse
V. Tjon B. Vogelaar

Project ID-Number : **CPD3259**
Date : June 19th 2001

HEAT EXCHANGER – SPECIFICATION SHEET

EQUIPMENT NUMBER	**:**	**E02**	**In Series**	**:**	1
NAME	**:**	**C01 Reboiler**	**In Parallel**	**:**	none

General Data

Service	:	- ~~**Heat Exchanger**~~ - ~~**Cooler**~~ - ~~**Condenser**~~	- ~~**Vaporizer**~~ - **Reboiler**
Type	:	- ~~**Forced Circulation**~~ - ~~**Kettle Reboiler**~~ - **Thermosyphon**	
Position	:	- ~~**Horizontal**~~ - **Vertical**	

Capacity	**[kW]**	**:**	6,354		**(Calc.)**
Heat Exchange Area	**$[m^2]$**	**:**	235.5		**(Calc.)**
Overall Heat Transfer Coefficient	**$[W/m^2 \cdot K]$**	**:**	950	*(1)*	**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[K]**	**:**	28.4		
Passes Tube Side		**:**	1		
Passes Shell Side		**:**	1		
Correction Factor LMTD (min. 0.75)		**:**	1.00		
Corrected LMTD	**[K]**	**:**	28.4		

Process Conditions

			Shell Side	**Tube Side**
Medium		**:**	C_7/C_8	LP steam
Mass Stream	**[tonne/day]**	**:**	1871.2	240.4
Mass Stream to				
- Evaporize	**[tonne/day]**	**:**	1871.2	-
- Condense	**[tonne/day]**	**:**	-	240.4
Average Specific Heat	**[kJ/kg· K]**	**:**	-	2.074 *(2)*
Heat of Evap. / Condensation	**[kJ/kg]**	**:**	293.4	2283.1
Temperature IN	**[K]**	**:**	397.5	463.0
Temperature OUT	**[K]**	**:**	397.8	406.5
Pressure	**[bara]**	**:**	1.25	3.0
Material		**:**	CS	CS

Remarks:

(1) From Coulson & Richardson's Chemical Engineering, Volume 6, page 567-568

(2) Average specific heat of vapor

Designers :	E. van Kints	M. Rijkse	Project ID-Number	:	**CPD3259**
	V. Tjon	B. Vogelaar	Date	:	June 19th 2001

HEAT EXCHANGER – SPECIFICATION SHEET

EQUIPMENT NUMBER	**:**	**E01**	**In Series**	**:**	1
NAME	**:**	**C01 Overhead Condenser**	**In Parallel**	**:**	none

General Data

Service	:	**- ~~Heat Exchanger~~**	**- ~~Vaporizer~~**
		- ~~Cooler~~	**- ~~Reboiler~~**
		- Condenser (water cooled)	
Type	:	**- Fixed Tube Sheets**	**- ~~Plate Heat Exchanger~~**
		- ~~Floating Head~~	**- ~~Finned Tubes~~**
		- ~~Hair Pin~~	**- ~~Thermosyphon~~**
		- ~~Double Tube~~	**-**
Position	:	**- ~~Horizontal~~**	
		- Vertical	

Capacity	**[kW]**	:	5,905.4		**(Calc.)**
Heat Exchange Area	**[m^2]**	:	174.2		**(Calc.)**
Overall Heat Transfer Coefficient	**[$W/m^2 \cdot K$]**	:	600	*(1)*	**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[K]**	:	56.9		
Passes Tube Side		:	1		
Passes Shell Side		:	1		
Correction Factor LMTD (min. 0.75)		:	1.00		
Corrected LMTD	**[K]**	:	56.9		

Process Conditions

			Shell Side	**Tube Side**
Medium		:	Cooling Water	$C_6/C_7/C_8$
Mass Stream	**[tonne/day]**	:	6,156.3	2,179.6
Mass Stream to				
- ~~Evaporize~~	**~~[tonne/day]~~**	:	-	-
- Condense	**[tonne/day]**	:	-	646.83
Average Specific Heat	**[$kJ/kg \cdot K$]**	:	4.177	-
Heat of Evap. / Condensation	**[kJ/kg]**	:	-	325.6
Temperature IN	**[K]**	:	293.0	362.0
Temperature OUT	**[K]**	:	313.0	358.6
Pressure	**[bara]**	:	1	1
Material		:	CS	CS

Remarks:

(1) From Coulson & Richardson's Chemical Engineering, Volume 6, page 567-568

Designers :	E. van Kints	M. Rijkse	Project ID-Number	:	**CPD3259**
	V. Tjon	B. Vogelaar	Date	:	June 19th 2001

HEAT EXCHANGER – SPECIFICATION SHEET

EQUIPMENT NUMBER	**:**	**E10**	**In Series**	**:**	1
NAME	**:**	**M01 Heat Exchanger**	**In Parallel**	**:**	none

General Data

Service	**:**	**- Heat Exchanger** **- ~~Cooler~~** **- ~~Condenser~~**	**- ~~Vaporizer~~** **- ~~Reboiler~~**
Type	**:**	**- ~~Shell and Tube~~** **- Shell and Tube: Floating Head** **- ~~Gasketed Plate~~** **- ~~Welded Plate~~**	**- ~~Plate Fin~~** **- ~~Spiral~~** **- ~~Double Pipe~~** **- ~~Direct Contact~~**
Position	**:**	**- Horizontal** **- ~~Vertical~~**	

Capacity	**[kW]**	**:**	3,782		**(Calc.)**
Heat Exchange Area	**$[m^2]$**	**:**	23.1		**(Calc.)**
Overall Heat Transfer Coefficient	**[W/m^2 K]**	**:**	850	*(1)*	**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[K]**	**:**	192.5		
Passes Tube Side		**:**	1		
Passes Shell Side		**:**	1		
Correction Factor LMTD (min. 0.75)		**:**	1.00		
Corrected LMTD	**[K]**	**:**	192.5		

Process Conditions

			Shell Side	**Tube Side**
Medium		**:**	C_6/C_7	HP Steam
Mass Stream	**[tonne/day]**	**:**	1176.1	151.8
Mass Stream to				
- Evaporize	**[tonne/day]**	**:**	-	-
- Condense	**[tonne/day]**	**:**	-	151.8
Average Specific Heat	**[kJ/kg K]**	**:**	2.883	2.331 *(2)*
Heat of Evap. / Condensation	**[kJ/kg]**	**:**	-	2157.2
Temperature IN	**[K]**	**:**	360.0	683.0
Temperature OUT	**[K]**	**:**	458.0	522.0
Pressure	**[bara]**	**:**	10.0	40.0
Material		**:**	CS	CS

Remarks:

(1) From Coulson & Richardson's Chemical Engineering, Volume 6, page 567-568

(2) Average specific heat of vapor

Designers :	E. van Kints	M. Rijkse	Project ID-Number	:	**CPD3259**
	V. Tjon	B. Vogelaar	Date	:	June 19th 2001

REACTOR - SPECIFICATION SHEET

EQUIPMENT NUMBER : **R01**
NAME : **Reactor 1**

General Data

Service : reactor
Column Type : vertical

Volume **[m^3]** : 151
Column Diameter **[m]** : 3.7
Column Height/Length **[m]** : 14
Column Material : SS

Catalyst : yes / ~~no~~
Type : Pt/Hβ
Mean Particle Size **[mm]** : 3.0
Shape : spheres
Bed Voidage **[%]** : 50%

Heating : ~~yes~~ / no
Duty **[MW]** :
Area Coils **[m^2]** :
Area Jacket **[m^2]** :

Cooling : yes / ~~no~~
Duty **[MW]** : 0.99
Area Coils **[m^2]** :
Area Jacket **[m^2]** :

Process Conditions

Stream Details		**Feed**	**Exit**			
Temp.	**[K]**	: 471	: 473			
Pressure	**[bara]**	: 9.50	: 8.66			
Density	**[kg/m^3]**	:	:			
Mass Flow	**[t/d]**	: 1814	: 1814			

Composition	**mol%**	**wt%**	**mol%**	**wt%**						
Hydrogen	88.9	13.8	87.9	13.7						
Propane	0.0	0.0	1.0	3.5						
Isobutane	0.0	0.0	1.0	4.6						
n-C7	2.9	22.2	1.5	11.4						
2-MHx	3.1	24.1	2.7	20.9						
3-MHx	3.2	25.0	2.6	20.2						
2,2-DMP	0.0	0.0	0.7	5.7						
2,3-DMP	1.2	9.3	0.9	6.7						
2,4-DMP	0.0	0.1	0.8	6.0						
3,3-DMP	0.2	1.6	0.4	3.4						
3-EP	0.3	2.7	0.3	2.6						
2,2,3-TMB	0.0	0.0	0.0	0.4						
2,4-DMHx	0.1	1.0	0.1	1.0						

Remarks:
(1) V01= effective volume = 9.6 m^3 for residence time of 5 minutes
(2) V02= effective volume = 55.2 m^3 for residence time of 5 minutes
(3) SS = Stainless Steel; CS = Carbon Steel

Designers : E. van Kints M. Rijkse
V. Tjon B. Vogelaar
Project ID-Number : **CPD3259**
Date : June 19th 2001

MEMBRANE SEPARATION UNIT – SPECIFICATION SHEET

EQUIPMENT NUMBER : **M01** **In Series** **:** 1
NAME **:** **Product Separation Membrane** **In Parallel** **:** none

General Data

Type **:** **- ~~Shell & Tube~~**
- ~~Countercurrent Monolith~~
- Cross-flow Monolith

Position **:** **- Horizontal**
- ~~Vertical~~

Mode **:** **- ~~Gas Permeation~~**
- Pervaporation

Mass Transfer **[t/d]** **:** 956 **(Calc.)**
Membrane Area **[m^2]** **:** 20,000 **(Calc.)**
Permeance (Mass Transfer Coefficient) [mol/m^2·s·Pa]: $1.0\cdot10^{-8}$ *(1)*
Pressure Difference **[bar]** **:** 9.0
Membrane Material **:** ZSM-5 (MFI) supported on monolith

Process Conditions

Stream Details	**Feed**		**Retentate**		**Sweep Gas**		**Permeate**		**~~Side Stream~~**	
Temp. [K]	: 458		: 458		: 504		: 473			
Pressure [bara]	: 10.0		: 10.0		: 1.00		: 1.00			
Density [kg/m^3]	:		:		:		:			
Mass Flow [t/d]	: 1176		: 220		: 77		: 1033			
Composition	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**
Hydrogen	0.0	0.0	0.0	0.0	100	100	80.0	7.5		
n-C6	1.4	1.2	0.0	0.0	0.0	0.0	0.3	1.4		
n-C7	3.0	3.0	0.0	0.0	0.0	0.0	0.7	3.4		
2-MHx	26.6	26.6	0.0	0.0	0.0	0.0	6.5	30.3		
3-MHx	16.8	16.8	0.0	0.0	0.0	0.0	4.1	19.2		
2,2-DMP	8.6	8.6	46.1	46.1	0.0	0.0	0.0	0.0		
2,3-DMP	10.5	10.5	0.0	0.0	0.0	0.0	2.6	12.0		
2,4-DMP	21.8	21.8	0.0	0.0	0.0	0.0	5.4	24.9		
3,3-DMP	6.4	6.4	34.0	34.0	0.0	0.0	0.0	0.0		
3-EP	1.2	1.2	0.0	0.0	0.0	0.0	0.3	1.4		
2,2,3TMB	3.7	3.7	19.8	19.8	0.0	0.0	0.0	0.0		
2,4-DMHx	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0		

Remarks:
(1) For the slowest permeating components (2,3-DMP and 2,4-DMP).

Designers :	E. van Kints	M. Rijkse	Project ID-Number	:	**CPD3259**
	V. Tjon	B. Vogelaar	Date	:	June 19th 2001

APPENDIX 18: DOW FIRE & EXPLOSION INDEX

Appendix Table 11: Estimation of material factors.

Compound	Flash point		Tb	NFPA ratings (0-4)			MF
	°F	°C	°C	N_F	N_R	N_H	
Hydrogen	Flammable gas		-252.60	4	0	0	21
Propane	Flammable gas		-42.07	4	0	1	21
Isobutane	Flammable gas		-11.73	4	0	1	21
n-C6	-9.4	-22.0	68.70	3	0	1	16
2-MP	20.0	-32.0	60.20	3	0	1	16
3-MP	19.4	< -20	63.20	3	0	1	16
n-C7		-4.0	98.50	3	0	1	16
2-MHX	26.6	-3.0	90.00	3	0	0	16
3-MHX	26.6	-3.0	92.00	3	0	0	16
2,2-DMP			79.20				
2,3-DMP	21.2	-6.0	89.70	3	0	0	16
2,4-DMP			80.40	3	0	0	16
3,3-DMP	21.2	-6.0	86.00	4	0	0	21
3-EP			93.50				
2,2,3-TMB			80.80				
2-MHEPT		4.4	117.60	3	0	0	16
3-MHEPT			118.90				
4-MHEPT	39.2	4.0	117.70	*3*	*0*	*0*	*16*
2,3-DMHX			115.60				
2,4-DMHX	37.4	3.0	109.50	*3*	*0*		*16*

Legend:

white cells	Data from literature
▨ shaded cells	Data from manufacturers
italic text	Estimated data

Appendix Table 12: Fire & Explosion Index sheet

Fire & Explosion Index Sheet

Area/Country:	**Division:**	**Location**	**Date**
Site	**Manufacturing Unit** Heptane isomerization plant	**Process Unit** F 01	

Materials in Process Unit

H2 n-C6 2-MP 3-MP N-C7 2-MHx 3-MHx 2,2-DMP 2,3-DMP 2,4-DMP 3-EP

State of Operation	**Basic Materials for Material Factor**
Design Start up X Normal Shutdown	All materials

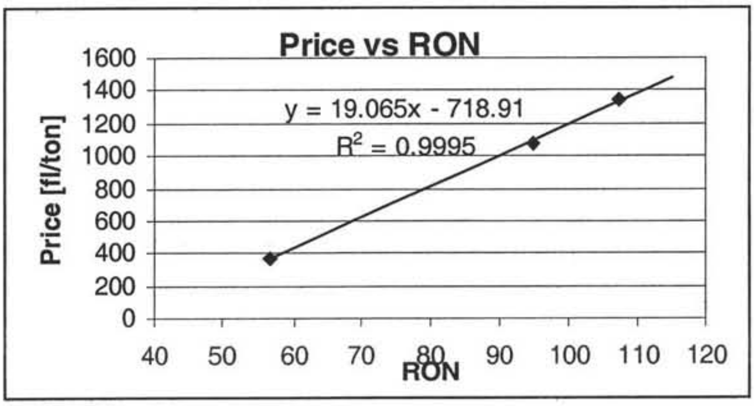
Material Factor (note requirements when unit temperature over 140 °F (60 °C)			21
1. General Process Hazards		**Penalty Factor Range**	**Penalty Used**
Base Factor		1.00	1.00
A. Exothermic Chemical Reactions		0.30 - 1.25	-
B. Endothermic Processes		0.20 - 0.40	-
C. Material Handling and Transfer		0.25 - 1.05	-
D. Enclosed or Indoor Process Units		0.25 - 0.90	-
E. Access		0.20 - 0.35	-
F. Drainage and Spill Control		0.25 - 0.50	0.50
General Process Hazards Factor (F1)			**1.50**
2. Special Process Hazards		**Penalty Factor Range**	**Penalty Used**
Base Factor		1.00	1.00
A. Toxic Material(s)		0.20 - 0.80	0.20
B. Sub-Atmosferic Pressure (< 500 mm Hg)		0.50	-
C. Operation In or Near Flammable Range			
1. Tank Farms Storage Flammable Liquids		0.50	-
2. Process Upset or Purge Failure		0.30	0.30
3. Always in Flammable Range		0.80	-
D. Dust Explosion		0.25 - 2.00	-
E. Pressure	Operating Pressure 1000 kPa Relief Setting - kPa		0.37
F. Low Temperature		0.20 - 0.30	-
G. Quantity of Flammable Material:	Quantity lb Hc = 1.91E+04 BTU/lb		
1. Liquids or Gases in Process			0.00
2. Liquids or Gases in Storage			-
3. Combustible Solids in Storage, Dust in Process			-
H. Corrosion and Erosion		0.10 - 0.75	0.10
I. Leakage - Joints and Packing		0.10 - 1.50	-
J. Use of Fired Equipment			1.00
K. Hot Oil Heat Exchange System		0.15 - 1.15	-
L. Rotating Equipment		0.50	-
Special Process Hazards Factor (F2)			**2.97**
Process Units Hazards Factor (F1 x F2) = F3			**4.45**
Fire and Explosion Index (F3 x MF = F&EI)			**93.46**

APPENDIX 19: PRICES BASED ON RON- NUMBER

For the estimation of the product and by-product prices the following prices given in Table 0-1 are used. With these prices a relation between RON number and price is made.
This relation is:
Price = 19.065 *RON – 718.91

Table 0-1. Gasoline prices.

	RON	Price fl/ton
Our Feed	57	365
gasoline	95	1080
ethylbenzeen	108	1340



With the relation the prices which are used in the design are given in Table 0-2.

Table 0-2. Product and by-product prices.

	RON	Price Fl/ton
our feed	56.7	362.08
Purge	40.6	55.13
Heavy	82.4	852.05
our product	92	1035.07

APPENDIX 20: ECONOMIC EVALUATION

Table 1. Maximum allowable investment at a interest rate of 10%

Year	NCF Mfl/a	NFW Mfl/a	DCF @ DCFROR 10% Mfl/a	Accumulative DCF Mfl/a
1		0.0	0.00	0.0
2		0.0	0.00	0.0
3	4.65	4.6	3.49	3.5
4	4.65	9.3	3.17	6.7
5	4.65	13.9	2.88	9.5
6	4.65	18.6	2.62	12.2
7	4.65	23.2	2.38	14.6
8	4.65	27.9	2.17	16.7
9	4.65	32.5	1.97	18.7
10	4.65	37.2	1.79	20.5
11	4.65	41.8	1.63	22.1
12	4.65	46.5	1.48	23.6
Maximum allowable Investment			23.6	Mfl

Table 2. DCF analysis

Net present and future worth and discount cash-flow						
Year	Capital cost Mfl/a	Cum. capital cost Mfl/a	NCF Mfl/a	NFW Mfl/a	DCF Mfl/a	NPW Mfl/a
0						
1	-44.29	-44.3	-44.3	-44.3	-40.27	-40.27
2	-44.29	-88.6	-44.3	-88.6	-36.61	-76.87
3			4.6	-83.9	3.49	-73.38
4			4.6	-79.3	3.17	-70.21
5			4.6	-74.7	2.88	-67.33
6			4.6	-70.0	2.62	-64.70
7			4.6	-65.4	2.38	-62.32
8			4.6	-60.7	2.17	-60.15
9			4.6	-56.1	1.97	-58.18
10			4.6	-51.420	1.79	-56.39
11			4.6	-46.774	1.63	-54.76
12			4.6	-42.128	1.48	-53.28
					-53.28	

At an interest rate at -9.5% the discount cash-flow is after 10 years of operation zero, this is shown in table 3.

Table 3. determining interest rate, so that NPW is zero.

Net present and future worth

Year	Capital cost	Cum. Cap. Cost	NCF	NFW cum. NCF	DCF @ DCFROR 9.5%	NPW cum.DCF
	Mfl/a	Mfl/a	Mfl/a	Mfl/a	Mfl/a	Mfl/a
1	-44.29455	-44.3	-44.3	-44.3	-48.994	-48.994
2	-44.29455	-88.6	-44.3	-88.6	-54.193	-103.187
3			4.6	-83.9	6.287	-96.900
4			4.6	-79.3	6.955	-89.945
5			4.6	-74.7	7.693	-82.253
6			4.6	-70.0	8.509	-73.744
7			4.6	-65.4	9.412	-64.332
8			4.6	-60.7	10.410	-53.922
9			4.6	-56.1	11.515	-42.407
10			4.6	-51.420	12.737	-29.671
11			4.6	-46.774	14.088	-15.583
12			4.6	-42.128	15.583	0.000
					0.000	

APPENDIX 21: DETAILED PROCESS DESCRIPTION OF C5/C6

Catalyst types

Three catalyst types are used for light naphtha isomerization: zeolitic catalysts, amorphous chlorided alumina catalysts and platinum supported on metal oxide.

Zeolitic Catalyst

This catalyst is a platinum loaded mordenite zeolite and does not contain a halide activator or promoter. The catalyst was originally developed by Shell for use in the Hysomer Process and was licensed by Union Carbide as part of their Total Isomerization Process (TIP). The zeolitic catalyst requires and operating temperature of around 260 °C and an operating pressure in the range of 18-35 bar.

Chlorided Alumina Catalyst

The UOP Penex catalyst is the highest activity isomerization catalyst commercially available today for C_5/C_6 isomerization. This high activity catalyst allows operation at a low temperature (120-180 °C), which thermodynamically favours the formation of branched isomers.
This high activity also results in a close approach to thermodynamic equilibrium. This high activity and low operating temperature results in improved product octane numbers and yields compared with the zeolite catalyst. Catalyst activity is maintained by the constant addition of organic chloride.

Metal Oxide Catalyst

Metal Oxides form the basis of a new generation of isomerization catalysts and is used in the ParIsom process. The development of this catalyst was based on a composition patented by Cosmo Oil Company Ltd. and Mitsubishi Heavy Industries Ltd. Japan.
The activity of this catalyst is considerably higher tan zeolitic catalysts, equivalent to about 80 °C in reactor temperature. This lower reaction temperature allows for significantly higher RON, 2-3 numbers higher tan a zeolitic catalyst.
The catalyst is fully regenerable using a simple oxidation procedure comparable to that practiced for zeolitic catalysts.

Recycle and Separation

In order to recycle the unconverted n-paraffins and single-branched isomers, these compounds must be separated form double-branched isomers. Separation can be carried out by distillation in large, energy-intensive columns, or by adsorption on molecular sieves.

Recycling with distillation

Various recycle flow schemes can be proposed. High octane numbers of up to 91 can be achieved even with zeolitic catalysts thanks to complex process flow schemes involving several distillation columns. However, these octane results will obviously be at the expense of process economics. The flow diagram giving the best RON/cost compromise includes a deisohexanizer (DIH) and leads to an octane number of 88, whatever the catalyst used. The richer the feed is in C_6, the more advantageous this set up is.

Recycling with adsorption on molecular sieves

IsoSiv

This separation process is developed by Union Carbide and uses molecular sieves to separate iso- and normal paraffins. The complete process operates in the vapor phase. The most common version of the IsoSiv process uses a difference in pressure between adsorption and desorption

(pressure swing) at temperatures between 200-300 °C. When the process is used as part of the Hysomer process, desorption is done by stripping with hydrogen.
The IsoSiv process operates with multiple beds (3-4), that are in adsorption or desorption mode.

Molex
An other process, used for separation of iso- and normal paraffins by use of molecular sieves, is a process developed by UOP. This process operates in the liquid phase and uses n-butane to desorp the adsorbed normal paraffins. N-butane can easily be separated from the paraffins by distillation. Because the separation method of the Molex process can be compared with chromatographic separations, the process can operate continuously.

IPSORB/HEXSORB
IFP has recently developed two molecular sieve separation processes: IPSORB and HEXOB. They are unique in that they integrate a distillation and a molecular sieve adsorption section: a deisopentanizer and molecular sieve desorption with iso-pentane for IPSORB, a deisohexanizer with methylpentanes desorption for HEXORB.
The aim of these process combinations is to:
Lower the n-paraffin content in the isomerate by desorption on a molecular sieve;
Raise the n-paraffin content in the feed by adding a separation column before the reaction section.
Additionally, since the temperatures in the reaction and separation sections are independent, all types of catalyst can be used in the reaction section.

PROCESS DESCRIPTIONS

In this paragraph, a detailed description of the processes found in Table 2-1 is given.

Penex
The Penex Process uses the highest activity chlorided alumina catalyst and, therefore, operates at lower temperatures (120-180 °C) than the Par-Isom or zeolitic isomerization processes. Due to the low operating temperature of the reactors, cracking reactions are minimal and there is no significant coke laydown on the catalyst. This enables the reactors to be run at a low Hydrogen/Hydrocarbon ratio, which removes the need for recycle gas separation. So no coolers, separators and recycle gas compressors are needed. The process uses molecular sieve driers to dry both the hydrocarbon feed and the Make-up gas. The driers are crucial to the Penex process since water is a permanent poison for the catalyst.
Two reactors are employed; when the catalyst in the first reactor needs to be replaced, the unit can operate on the second reactor only. In normal operation the second rector runs at a lower temperature to establish a more favorable equilibrium [27]

Penex/DIH Recycle
In this scheme a deisohexanizer (DIH) fractionates the stabilized isomerate product producing an overhead isomerate product containing all the C_5s and dimethylbutanes. N-C_6 and some of the methylpentanes are taken as a side-cut form the column and are recycled back to the reactor. The small bottoms drag stream contains the heavy portion of the product (C_7+ material and some C_6 cyclics) which can be sent to gasoline blending or the reformer.
The recycled n-C_6 and methylpentanes are further isomerized to high octane dimethylbutanes which particularly boosts the motor octane number of the product. A draw-back with this system is that the C_5s are only isomerized in a single pass and thus the process is predominantly attractive for C_6 feeds.

Penex/Molex Recycle
In this process a Gasoline Molex Unit is used to separate the is-paraffins from the normal paraffins with the normals being recycled back to the Penex reactors. The high activity of the Penex catalyst combined with the high efficiency separation of the Molex process enables the

Penex reactors to be run at a higher space velocity than the other Penex flowschemes. This reduces the amounts of catalyst and platinum.

Isomerization Process BP [28]

The isomerization process of British Petroleum is strongly related to the Penex process. Similarities can be found in the type of catalyst and therefore same restrictions towards sulfur and water contents of the feeds and the use of two reactors. HCl is recycled to maintain the amount of chloride of the catalyst.

Zeolitic Isomerization [27]

The flowscheme is simple. Typically containing a single reactor, a charge heater, coolers, separator, recycle gas compressor and stabilizer column. The isomerization takes place in the vapor phase at relatively low pressures of approximately 15 to 35 bar, temperatures ranging between 200 and 340 °C and in the presence of hydrogen [26]. The feed is combined with recycled hydrogen and heated to operating temperature before entering the reactor. From here, the equilibrium mixture is cooled and passed to a separator, from which hydrogen is recycled. The liquid isomerate passes to a stabilizer to remove small amounts of PLG formed in the reaction. Any benzene in the feed is saturated to cylohexane, which, in turn, is partly converted to paraffins.

TIP [27].

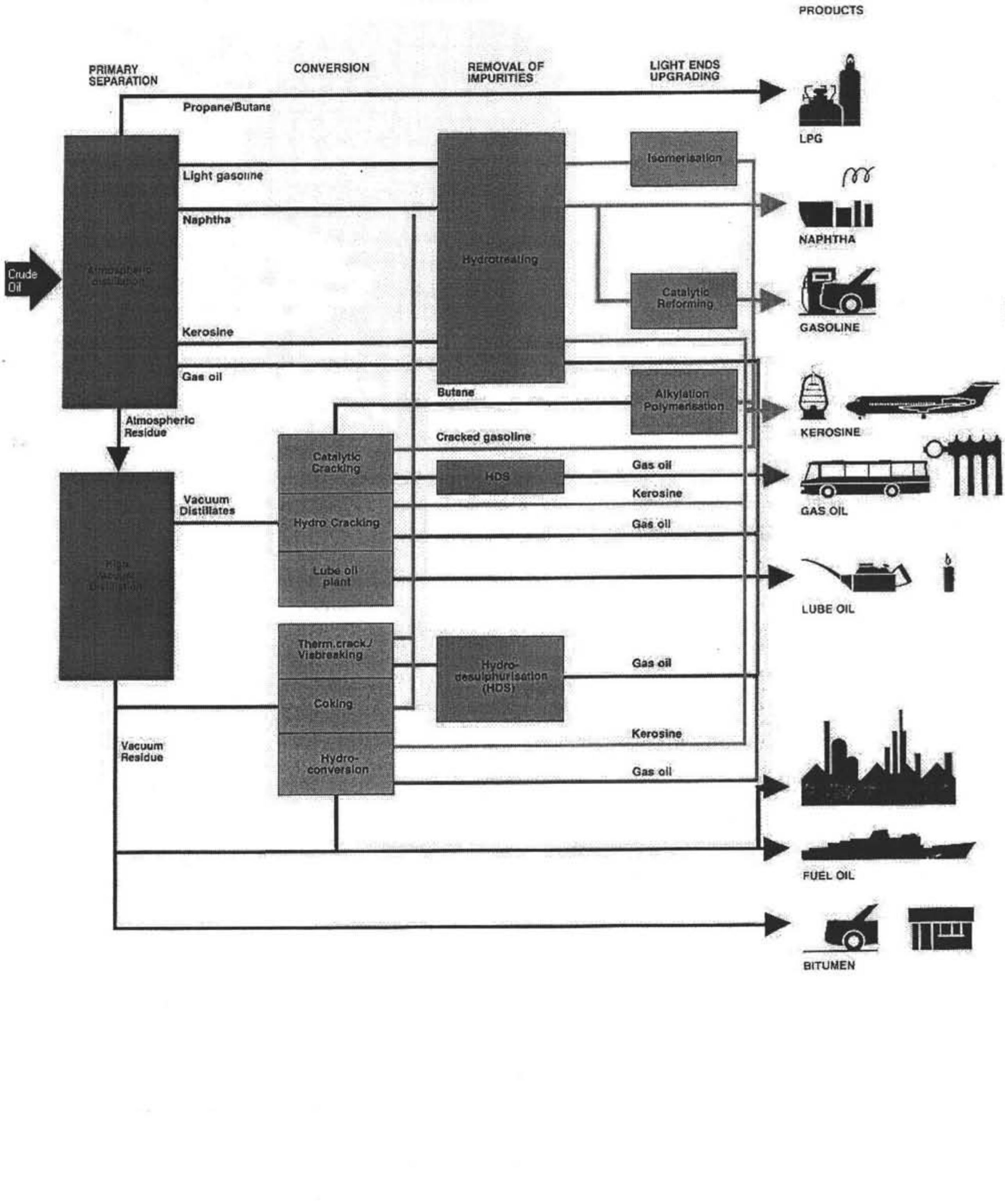
The Total Isomerization Process is the integration of the once through hydrocarbon Zeolitic Isomerization Process with the IsoSiv molecular sieve adsorption process for the separation and recovery of normal paraffins. Extensive integration of the two processes is made possible by use of similar operation conditions (temperature and pressure).

The IsoSiv Process has typically 4 adsorbers in a TIP unit. The molecular sieves themselves are of a controlled-pore size that will allow straight-chain n-paraffins to enter, but no the wider branched-chain isoparaffins. A desorption step (the n-paraffins adsorbed on the sieve are desorbed by means of hot hydrogen [26]), following the adsorption cycle allows recovery of the n-paraffins for recycle to the isomerization reactor. The separation and recycle of normal paraffins back to the Isomerization reactor allows a much higher octane number of the product to be attained than form a once trough unit.

Par-Isom Process

This process represents the latest innovation in light naphtha Isomerization. The key is a high performance metal oxide catalyst, with activity approaching that of chlorided alumina catalysts that is both robust and regenerable. The process flow scheme is similar to that used for conventional zeolitic isomerization units. The fresh C_5/C_6 feed is combined with make-up and recycle hydrogen and this is directed to a charge heater, where the reactants are heated to reaction temperature. A fired heater is not required in the Par-Isom process during normal operation, due to the much lower reaction temperature needed with the metal oxide catalyst compared to a zeolite catalyst. Hot oil or steam can be used for the heat source in this exchanger. The availability of a fired heater is required, however, for catalyst regeneration (every 18 months-2 years). The heated combined feed is then sent to the reactor. Either one or two reactors can be used in series.

APPENDIX 22: OIL REFINERY SCHEME



APPENDIX 23: STOICHIOMETRIC REACTIONS

I. Linear

[1]

[2]

II. Monomethyl

[3]

[4]

[5]

[6]

b. 3-methylhexane

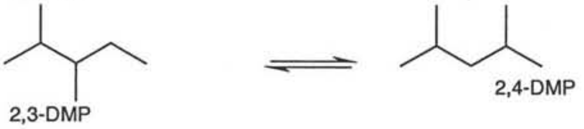
[7]

[8]

[9]

III. dimethylpentane

[10]



[11]

[12]

[13]

APPENDIX 24: PURE COMPONENT S

PURE COMPONENT PROPERTIES

Component Name		Technological Data							Medical Data		Notes
Design	Systematic	Formula	Mol. Weight g/mol	RON	Boiling Point (1) °C	Melting Point (1) °C	Density of Liquid (2) kg/m³	Density of Gas (3) kg/m³	MAC value ppm	LD50 Oral (4) g	
H2	Hydrogen	H_2	2.016		-252.60	-259.14	24.1	0.082			(5)
C-1											
meth	methane	CH_4	16.043	>120	-161.50	-182.48	117.0	0.657			(5)
C-2											
eth	ethane	C_2H_6	30.070	118	-88.63	-182.80	284.0	1.240			
C-3											
prop	propane	C_3H_8	44.097	112	-42.07	-187.69	512.0	1.830	1000		
C-4											
but	butane	C_4H_{10}	58.123	93	-0.45	138.29	602.0	2.440			
i - but	2-methyl propane	C_4H_{10}	58.123	99	-11.73		582.0	2.440			
C-5											
n - pent	n-Pentane	C_5H_{12}	72.150	62	36.30	-129.73	630.0	liquid	600		
i - pent	Iso-pentane	C_5H_{13}	72.150	93	27.95	-160.00	621.0	liquid			
C-6											
n - hex	n-hexane	C_6H_{14}	86.177	29	68.70	-95.30	654.8	liquid	25		
2 MP	2-methylpentane	C_6H_{14}	86.177	78	60.20	-153.70	650.0	liquid	200		
3 MP	3-methylpentane	C_6H_{14}	86.177	76	63.20	-162.90	659.8	liquid	200		
2,2 DMB	2,2-dimethylbutane	C_6H_{14}	86.177	92	49.70	-99.00	644.4	liquid	200		
2,3 DMB	2,3-dimethylbutane	C_6H_{14}	86.177	104	57.90	-128.80	661.6	liquid	200		
C-7											
n-hept	n-heptane	C_7H_{16}	100.204	0	98.50	-90.60	684.0	liquid	500		(4)
2 MHx	2-methylhexane	C_7H_{16}	100.204	42	90.00	-118.20	679.0	liquid			(4)
3 MHx	3-methylhexane	C_7H_{16}	100.204	52	92.00	-119.00	686.0	liquid			
3 EP	3-ethylpentane	C_7H_{16}	100.204	65	93.50	-118.60	698.0	liquid			
2,2 DMP	2,2-dimethylpentane	C_7H_{16}	100.204	93	79.20	-123.80	674.0	liquid			(4)
2,3 DMP	2,3-dimethylpentane	C_7H_{16}	100.204	91	89.70		695.0	liquid			
2,4 DMP	2,4-dimethylpentane	C_7H_{16}	100.204	83	80.40	-119.90	673.0	liquid			
3,3 DMP	3,3-dimethylpentane	C_7H_{16}	100.204	81	86.00	-134.90	694.0	liquid			
2,2,3 TMB	2,2,3-trimethylbutane	C_7H_{16}	100.204	109	80.80	-25.00	690.0	liquid			
C-8											
n - oct	n-octane	C_8H_{18}	114.230	<0	125.60	-56.80	699.0	liquid	500		(6)
2 MHp	2-methylheptane	C_8H_{18}	114.230	22	117.60	-108.90	698.0	liquid			(6)
3 MHp	3-methylheptane	C_8H_{18}	114.230		118.90	-120.00	707.5	liquid			
4 MHp	4-methylheptane	C_8H_{18}	114.230		117.70	-121.00	704.6	liquid			
2,2 DMHx	2,2-dimethylhexane	C_8H_{18}	114.230	73	106.80	-121.10	695.3	liquid			(6)
2,3 DMHx	2,3-dimethylhexane	C_8H_{18}	114.230		115.60		691.2	liquid			
2,4 DMHx	2,4-dimethylhexane	C_8H_{18}	114.230		109.50		696.2	liquid			
2,5 DMHx	2,5-dimethylhexane	C_8H_{18}	114.230		109.10	-91.00	690.1	liquid			

Notes:

- (1) At 1 atm
- (2) At 25°C
- (3) At 25°C, 1 atm
- (4) Oral in g 's for a male of 70 kg's weight
- (5) Density of liquid at critical point
- (6) Source RON [16]

Source: [7], [9] shaded areas

Project ID Number :	**CPD3259**
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APPENDIX 25: CATALYSTS DATA

Table 0-3 shows the literature data for the hydroisomerization of n-heptane found for various isomerisation catalysts:

Table 0-3: n-Heptane isomerization catalysts

Catalyst	T(K)	P(bar)	Conv.(%)	Sel. Mono(%)	Sel. Multi(%)	Ref.
Se CoHZSM5	533	20	10.0	20.1	2.4	1
SAPO-11	653		74.2	69.1	24.1	2
MoO3	523/398	1.1	81.2	67.6	21.5	3
Pt/USY	523	1.1	74.0	83.4	5.8	3
MoO3	623		18.8	74.5		4
Pt/Beta	533	30	66.6	36.9	9.0	5
Pd/SAPO-11	573	3				6
Pt/Hbeta	**483**	**1**	**83.9**	**60.0**	**26.1**	**7**
Pt/CaY	673	2.3	72.0	49.8	18.4	8
PtPd/H-USY	505	3	82.5			9
Pt/H-beta	500		82.5	70.0		10

As the objective for the first reactor stage is to generate a high amount of multibranched isomers, the Pt/Hbeta catalyst was chosen for its high selectivity and stability.

Table AII-2: Catalyst 1 conversion (data wt%)

lit	Catalyst	2MH	3MHx	3EP	2,2-DMP	2,3-DMP	2,4-DMP	3,3-DMP	2,2,3-TMB	Cracking	feed
7	Pt/Hbeta	25	24.1	0.4	5.9	6.6	6.4	2.1	0.5	13.90	H2/C7 =18

Table AII: 1.3: Catalyst 2 conversion data [11]
Catalyst : Si-Al 5w% Ni
P= 24.8 atm
T=316°C
LHSV=1.0 v/v/h
H2/HC=4 (molar ratio)

Table AII-3. Catalyst 2 conversion data of 4 components to the other components

Load	Conversion	Yield Isomer	n-C7	2MHx	3MHx	3EP	2,2-DMP	2,3-DMP	2,4-DMP	3,3-DMP	2,2,3-TMB	Cracking
n-heptane	19.7	18.7		6.3	9	0	0	0	3.4	0	0	1
2,3 DMP	54.5	49.3		27.92	30.14	2.15	0.98	3.45	2.09	0.57	0.03	50.3
2,4-DMP	75.2	69.9	1.9	11.3	12	0.8	0	22.7	0	8.2	13	5.4
2,2,3 TMB	18	17.1					8.5	4.7	3.9			0.9

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APPENDIX 26: UTILITY CONDITIONS AND COSTS

1. Available Utilities

a. Steam

Superheated steam is considered to be available at the temperatures and absolute pressures given below.

Conditions	Steam Class		
	High Pressure	Medium Pressure	Low Pressure
p [Bara] :	40	10	3
T (superheated) [°C)] :	410	220	190
T (condensation) [°C)] :	250	180	133.5

b. Electricity

Power	Voltage [V]	Current
Low :	220	AC
Medium :	380	three-phase AC
High :	3000 – 10000 (3 – 10 kV)	three-phase AC

c. Water

Water	T [°C]		p[Bara]	h [kW/m^2 °C]?	Fouling factor [m^2 °C/kW]
	in	out			
Potable :	15		4		
Demineralized (process) :	15		7		
Cooling :	$20^{(1)}$	$40^{(2)}$	$3^{(3)}$	2.0	0.5
Remarks :	(1)	Design value			
	(2)	Maximum allowed			
	(3)	At ground level			

2. Utility Costs

UTILITY COSTS, EXCL. VAT[1]

Utility	Units[2]		LHV	Unit Costs, Nfl/unit			
	Quant.	Energy	En. per Quant.	Quant.		Energy	
				Min.	Max.	Min.	Max.
NG[3,4]	Nm^3	MJ	31.65	0.26	0.43	0.00821	0.013586
	kg	MJ	37.68	0.31	0.51	0.00821	0.013586
	ton	MJ	37678.57	309.52	511.90	0.00821	0.013586
HFO[5]	ton	MJ	41.45	280.00	300.00	6.75513	7.237636
Coal	ton	MJ	29.30	110.00		3.75427	0
Steam LP/HP	ton			30.00	35.00		
Electricity[6]		kWh				0.13	0.22
Cooling Water	m^3			0.05	0.10		
BFW/Process W.	m^3			1.10	2.50		
Presurized Air[7]	Nm^3			0.05			

Remarks

1. Ref. "Cost Data, WEBCI / DACE", 18th Edition November 1995
2. 1 ton = 1000 kg
3. NG = natural gas
4. Density : 0.84 kg/Nm^3 , MW : 18.60
5. HFO = heavy fuel oil
6. For quantities larger than 10^6 kWh/a
7. Air pressure 7 Bara

APPENDIX 27: CALCULATION FOR REFLUX ACCUMULATOR VESSEL

Assumptions:

- Residence time (liquid) of 5 minutes
- Liquid level at 50% of height
- L/D ratio is 4

The residence time τ [s] is:

$$\tau = \frac{V_{vessel,effective}}{\Phi_{V,liquid}}$$

where: $V_{vessel,effective}$ = effective volume of accumulation vessel [m^3]
$\Phi_{V,liquid}$ = volumetric flow rate liquid [m^3/s]

The volumetric liquid flow rate can be calculated with

$$\Phi_{V,liquid} = \frac{\dfrac{\Phi_{m,liquid} \bullet 1000}{24 \bullet 3600}}{\rho_L}$$

where: $\Phi_{m,liquid}$ = mass flow rate liquid [t/d]
ρ_L = density of liquid [kg/m^3]

The effective volume of the collection vessel $V_{vessel,effective}$ can be calculated with:

$$V_{vessel,effective} = \Phi_{V,liquid} \bullet \tau = \frac{\dfrac{\Phi_{m,liquid} \bullet 1000}{24 \bullet 3600}}{\rho_L} = \frac{\Phi_{m,liquid}}{\rho_L} \bullet 3.47$$

Take the actual volume of the vessel V_{vessel} twice $V_{vessel,effective}$:

$$V_{vessel} = 2 \bullet V_{vessel,effective} = \frac{\Phi_{m,liquid}}{\rho_L} \bullet 6.94$$

Assuming the L/D ratio of the vessel is equal to 4, the dimensions of the vessels can be calculated. The results are summarized in the table below.

Table: Summary of results for reflux accumulator vessels

	$V_{vessel,effective}$	V_{vessel}	D	L
V01	9.6	19.2	1.8	7.3
V02	55.2	110.4	3.3	13.1
V03	48.6	95.1	3.1	12.5