

Abstract

In the last years there have been much research and development regarding gas-to-liquid plants. The fuel demands are growing bigger, and fuels from oil and coal cannot cover the demands in the future. Converting natural gas to liquid fuels is a good way to fill the gap between supply and demand. The fuels from natural gas are cleaner than from oil and coal, because they contain less sulfur and aromatics.

In this thesis a gas to liquid plant using Fischer-Tropsch synthesis was investigated. The main focus was the hydrotreater. In the hydrotreater cracking and isomerization reactions took place. Aspen's simulation program HYSYS combined with Mathworks program MATLAB were used to solve the equations in the hydrotreater. After the simulation was done, an economic analysis of the whole plant was done using Microsoft Excel.

The optimal conditions for the hydrotreater were an inlet temperature and pressure of 335 °C and 25 bars. The H₂/wax ratio was 0.14 and the minimum reactor volume 33 m³. Recycling the light ends was found to be more profitable and carbon efficient than purging them.

The project seemed to be beneficial and the net present value was about 3.8 billion dollars over a 20 years horizon and 9% discount rate. The internal rate of return became 52%, and the return on investment 53%.

Oppsummering

I de siste årene har det vært gjort mye forskning og utvikling angående gass til væske anlegg. Behovene for drivstoff øker, og drivstoff fra olje og kull kommer ikke til å dekke behovene i fremtiden. Ved å konvertere naturgass til flytende drivstoff kan man fylle gapet mellom tilbud og etterspørse. Drivstoffene fra naturgass er dessuten renere enn de fra olje og kull, grunnet lavere svovel og aromat innhold.

I denne masteroppgaven var det et gass til væske anlegg som bruker Fischer-Tropsch syntese som ble undersøkt. Hovedfokuset lå på hydrogenbehandlingsreaktoren, hvor krakking og isomeriseringsreaksjoner fant sted. Aspen sitt simuleringsverktøy HYSYS ble kombinert med Matworks program MATLAB for å løse ligningene i hydrotreateren. Etter simuleringene var ferdig ble det gjort en økonomisk analyse av hele anlegget ved hjelp av Microsoft Excel.

De optimale betingelsene for hydrogenbehandlingsreaktoren var en innløpstemperatur på 335 °C og et innløpstrykk på 25 bar. Hydrogen/voks forholdet var 0,14 og det minste reaktorvolumet 33 m³. Ved å resirkulere de letteste komponentene tilbake ble det oppnådd bedre karboneffektivitet og bedre lønnsomhet.

Prosjektet så ut til å være lønnsomt, og nåverdi ble 3,8 milliarder dollar for et prosjekt med 20 års levetid og 9% diskonteringsrente. Internrenten for prosjektet ble 52% og avkastningen på investeringen ble 53%.

Pre face

This master thesis was written in the spring of 2012 in the subject TKP4900, environmental engineering and reactor technology, at the department of Chemical Engineering (IKP) at the Norwegian University of Science and Technology (NTNU). In this thesis Aspen's simulation program HYSYS was used (version 7.2), along with Mathworks numerical computing program MATLAB version R2010b and Microsoft Excel 2010.

Supervisor for the thesis was Professor Magne Hillestad. I would like to thank Magne for helping me and giving good advices during the project.

*"I declare that this is an independent work according to the exam regulations
of the Norwegian University of Science and Technology"*

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Trondheim 14.06.2012

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Abbreviations

ASF	Anderson-Schultz-Flory
ASU	Air Separation Unit
ATR	Auto Thermal Reforming/Reformer
CEPCI	Chemical Engineering's Plant Cost Index
CF	Cash Flow
CSTR	Continuous Stirred Tank Reactor
D&E	Design & Engineering
EOS	Equation Of State
FT	Fischer-Tropsch
GTL	Gas To Liquid
HP	High Pressure
HYSYS	Simulation program
IRR	Internal Rate of Return
ISBL	InSide Battery Limit
LHS	Left Hand Side
LP	Low Pressure
LPG	Liquefied Petroleum Gas
MATLAB	MATrix LABoratory
NOK	NOrwegian Krone
NPV	Net Present Value
OPEC	Organization of Petroleum Exporting Countries
OS	Off-Sites
OSBL	OutSide Battery Limit
PFM	Plug Flow Model
PFR	Plug Flow Reactor
POX	Partial OXidation
ppm	parts per million
RHS	Right Hand Side
ROI	Return On Investment
SR	Steam Reforming
ULSD	Ultra Low Sulfur Diesel
US	United States
VLE	Vapor Liquid Equilibrium
WGS	Water Gas Shift
X	Contingent

1. Introduction

The Fischer-Tropsch (FT) process is named after the two Germans, F. Fischer and H. Tropsch. They were the first to industrialize this process in the years 1925-1935. Before that two Frenchmen, Sabatier and Senderens, had described the main reaction for the process (1). The Fischer-Tropsch synthesis is a gas-to-liquid (GTL) process, where natural gas is converted into liquid fuels such as diesel. The Fischer Tropsch synthesis is good way to utilize stranded gas¹ (2).

1.1 General information

There are several GTL plants using the Fischer-Tropsch process. Among them are the ORYX plant in Qatar, which is owned by Qatar Petroleum and Sasol, which has a capacity of producing 34 000 bbl/day, the Shell Bintulu plant in Malaysia and the new PEARL project in Qatar (3). The PEARL project will operate at full production in 2012, and have a capacity of producing 140 000 bbl/day (4).

A GTL plant consists of three sections; syngas preparation, FT synthesis and upgrading of the products (2). The syngas production is most expensive. There are several processes for preparing the syngas; Steam reforming (SR), auto thermal reforming (ATR), partial oxidation (POX) or a combination of these (5). In the FT synthesis there is mainly two types of reactors being used; a slurry bubble column or a multitubular fixed bed reactor. The slurry bubble column reactor has been suggested because it is more isothermal, and is more appropriate for heat removal in the exothermic FT reaction (6).

There are two different FT syntheses, high and low temperature. The high temperature synthesis uses iron catalyst, operates at 330-350 °C and produces mainly light hydrocarbons (naphtha). The low temperature FT synthesis can use both cobalt and iron catalyst, operates at temperature around 200 °C and produces mainly heavier hydrocarbons (diesel and wax) (7).

The two main catalysts used in the Fischer-Tropsch reactor are cobalt and iron. There are several differences in the use of these two catalysts. The iron catalyst is used for the high-temperature synthesis, but both can be used for the low temperature synthesis. The iron catalyst produces more olefins, while the cobalt catalyst is more resistant to attrition and more suitable

¹ The gas reserve is too remote from a natural gas market, and making pipelines is too expensive

for slurry reactors. The cobalt catalyst operates at a narrow temperature interval, and a small change in temperature can significantly change the methane selectivity (8). A comparison between them is given in Table 1

Table 1 - Comparison of cobalt and iron catalyst (8)

Parameter	Cobalt	Iron
Cost	More expensive	Less expensive
Lifetime	Resistant to deactivation	Less resistant to deactivation
Activity at low conversion	Same as iron	Same as cobalt
Productivity at high conversion	Higher, less significant effect of water on the rate of CO conversion	Lower, strong negative effect of water on the rate of CO conversion
Maximum chain growth probability	0.94	0.95
WGS reaction	At high conversion	
Maximum sulfur content	< 0.1 ppm	< 0.2 ppm
Flexibility (temperature and pressure)	Less flexible	Flexible
H ₂ /CO ratio	~2	0.5-2.5
Attrition resistance	Good	Not very resistant

In the upgrading unit, the long hydrocarbon chains from the FT synthesis undergo hydrocracking and hydroisomerization reactions in a hydrotreater. Wax is cracked to get smaller hydrocarbon chains, since diesel is the wanted product. Isomerization improves the knocking properties, the cold properties and enhances the cetane number of the fuels (9) (10). Hydroisomerization implies that molecular structures are modified, which means that linear paraffins become branched paraffins. Hydroprocessing is used as a collective term for heterogenic reaction systems that include hydrogen, and include the terms hydrocracking and

hydroisomerization among others (9). Last part of the upgrading unit is fractionation of the fluid mixture. Fractionation is separation of a fluid into several smaller quantities, called fractions.

The fuels from Fischer-Tropsch synthesis are extremely clean. The diesel made from FT-synthesis has lower sulfur content than the new Ultra Low Sulfur Diesel (ULSD) made from petroleum (11). The sulfur content is less than 1 ppm, there are less than 1% aromatics, the diesel has high cetane number (70-80) and the energy density is 7% higher than regular fuel (7). All of these properties are good for diesel. The FT synthesis is not so good for making high quality gasoline because the aromatic content is too low (9).

There are several actors on the market which have licensed technologies for hydroprocessing hydrocarbon mixtures, Haldor-Topsøe and Chevron are two examples. These actors also have suitable catalysts for the process (9).

The catalysts used in the hydroprocessing reactor are bifunctional, containing a hydrogenation/dehydrogenation function and characterized by acidic sites to provide isomerization and cracking. Typical acidic supports are zeolites or crystalline/amorphous silica-alumina. The most common metals used are non-noble metal combinations like Ni/Mo, Co/Mo or noble metals like Pt and Pd (9), (12).

1.2 Project goals

This thesis is a continuation of a project done earlier (13). In the earlier project the syngas production and FT synthesis were investigated and optimized. In this project the upgrading unit is the main focus. Some of the values used in this report are derived from the earlier report which can be found in the Appendix F. In the past report the Steam/carbon and oxygen/carbon ratio into the ATR was investigated along with the FT reactor volume and the splits for stream 11 and 12 as seen from flowsheet on Figure 1. Heat integration was also done in the earlier report.

In this thesis a mathematical model for the hydrotreater shall be derived in a modelling program (MATLAB), and sent to a simulation program (HYSYS). The goals will be to get these two programs to cooperate, and find the optimal conditions for the hydrotreater. In addition an economic analysis for the entire plant shall be done.

2. Process Description

A typical process flow diagram for a GTL plant is illustrated in Figure 1. In this figure the Air Separation Unit (ASU) and hydrogen plant are not shown.

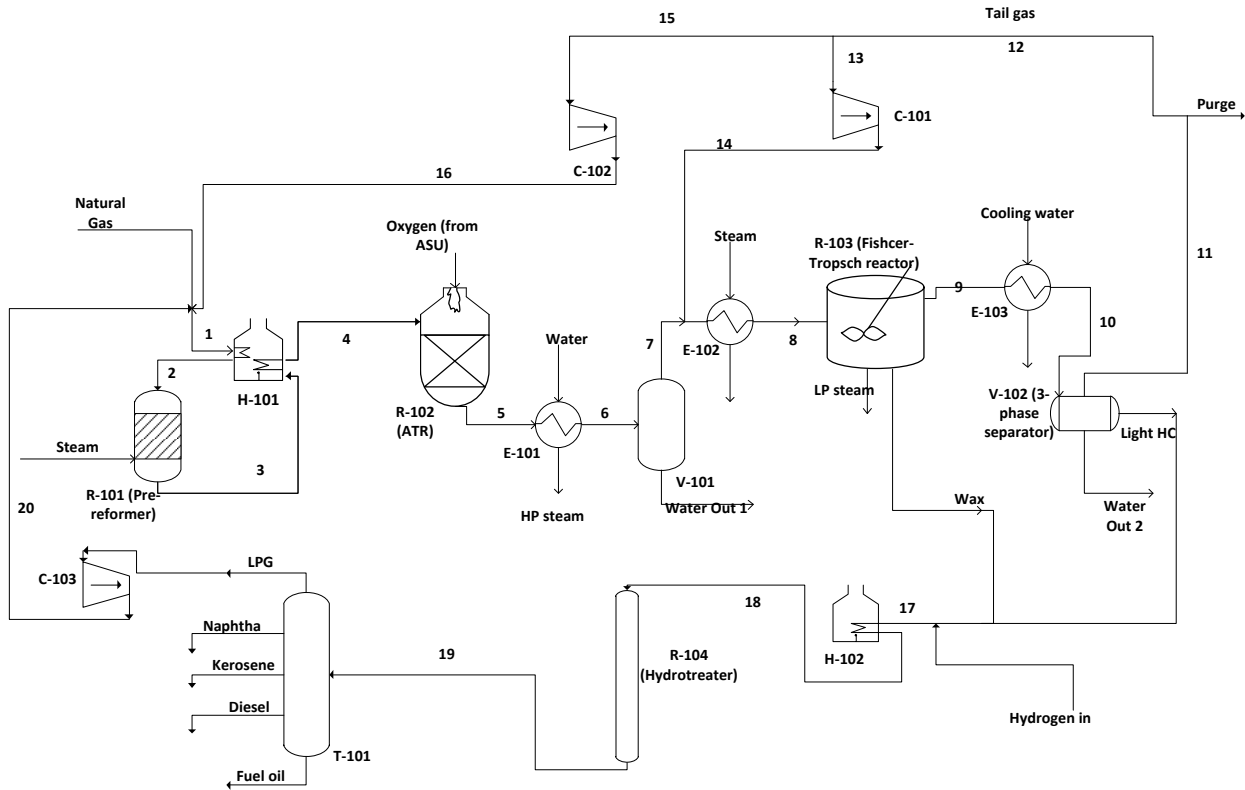


Figure 1 - Flowsheet for GTL plant

The inlet conditions (the stream named ‘Natural Gas’ on flowsheet) are given in Table 2. The inlet conditions used were given by supervisor (14).

Table 2 - Inlet Conditions

	Temperature	Pressure	Flow rate	Composition:	CH ₄	C ₂ H ₆	C ₃ H ₈	i-C ₄ (iso-butane)	i-C ₅ (iso-pentane)
Value	50 °C	50 bars	8218 kmole/h	Mole fractions	0.95	0.02	0.015	0.01	0.005

A summary of the most important streams from the syngas production and FT synthesis are given in Table 3. Steam, oxygen, hydrogen and product streams are given further down in the report. The subscripts i/n means iso and normal.

Table 3 - Stream properties

Stream name	2	3	4	5	6	8	9	10	Wax	11	Light HC	Purge	14	16
Temperature [°C]	455	458	650	1030	30	210	210	30	210	30	30	30	37	44
Pressure [bar]	30	30	29	29	28	27	27	26	27	26	26	26	28	30
Mass Flow [ton/h]	204	330	330	498	498	1508	1452	1452	56	1228	65	43	1138	47
Mass fractions														
ω_{nC1-4}	0.75	0.46	0.46	0.01	0.01	0.11	0.12	0.12	0.00	0.14	0.05	0.14	0.14	0.14
ω_{nC5-9}	0.01	0.00	0.00	0.00	0.00	0.01	0.03	0.03	0.01	0.02	0.32	0.02	0.02	0.02
ω_{nC10+}	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.02	0.98	0.00	0.53	0.00	0.00	0.00
ω_{iC5-9}	0.02	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
ω_{H_2O}	0.00	0.34	0.34	0.26	0.26	0.00	0.11	0.11	0.00	0.00	0.00	0.00	0.00	0.00
ω_{H_2}	0.01	0.01	0.01	0.07	0.07	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ω_{CO}	0.01	0.00	0.00	0.49	0.49	0.18	0.02	0.02	0.00	0.02	0.00	0.02	0.02	0.02
ω_{CO_2}	0.22	0.19	0.19	0.17	0.17	0.67	0.70	0.70	0.01	0.82	0.09	0.82	0.82	0.82
Sum	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

The mass fractions of oxygen and i-C₁₀₊ are not given in this table, because they were not present in these streams. The values were rounded and are thus not accurate. For more accurate values, or other property values such as mole flow, the HYSYS file given as an electronic appendix can be examined in Appendix F.

2.1 Syngas Production

The natural gas entered a fired heater to reach the desired temperature before entering an adiabatic pre-reformer. This temperature is normally between 350-550 °C (15). Water steam was added to the pre-reformer along with the heated natural gas. In the pre-reformer following reactions took place (2) (15). The enthalpies are given in [kJ/mole].



In the pre-reformer all higher hydrocarbons, except methane, were converted into CO and H₂ according to reaction 2.a. The hydrogen and carbon monoxide were brought into equilibrium with methane and water according to reaction 2.b. Reaction 2.c, which is the water-gas-shift (WGS) reaction, also took place in the pre-reformer.

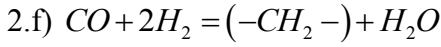
After the pre-reformer the gas was heated before it entered an oxygen blown ATR. The temperature of the inlet gas should be around 650 °C (15). The oxygen blown into the ATR should be around 200 °C (2). Inside the ATR there were three reactions (15).



After being reformed, the gas was cooled down, and water was removed in a separator. Then the syngas was heated to 180-250 °C (16) before it entered the FT reactor.

2.2 Fischer-Tropsch synthesis

In the FT-reactor the syngas reacted to form higher hydrocarbons according to reaction 2.f.



The catalyst used in this reactor was a cobalt catalyst, and the kinetic model used, was found in literature (17), and can be seen in equation 2.1.

$$r_{CO} = \frac{k_1 P_{H_2}^{0.6} P_{CO}^{0.65}}{1 + K_1 P_{CO}} , \left[\frac{kmole_{CO}}{m_{reactor}^3 s} \right] \quad (2.1)$$

Where the parameters k_1 and K_1 are given below

$$k_1 = 1.6 \cdot 10^{-5} \exp\left(-\frac{37326}{RT}\right) , \left[\frac{kmole_{CO}}{Pa^{1.25} m_{reactor}^3 s} \right] \quad (2.2)$$

$$K_1 = 1.096 \cdot 10^{-12} \exp\left(-\frac{-68401.5}{RT}\right) , [Pa^{-1}] \quad (2.3)$$

The kinetic model found in literature was given in mole per second and per gram surface metal. To convert the expression to the wanted units, some assumptions were made. The catalyst density was assumed to be 2000 kg/m^3 , the weight fraction of cobalt in catalyst was 20%, and 10% of the cobalt was exposed as surface atoms. The catalyst volume fraction was 10% (18).

To calculate the product distribution, there were assumed that the products followed the ideal ASF (Anderson-Schultz-Flory) distribution. The chain growth probability, α_{ASF} , was set constant to 0.9, even though it is actually an empirical correlation of partial pressures and temperature (19). The distribution can be seen in Figure 2. The value 0.9 was chosen because diesel was the wanted product cf. Figure 2.

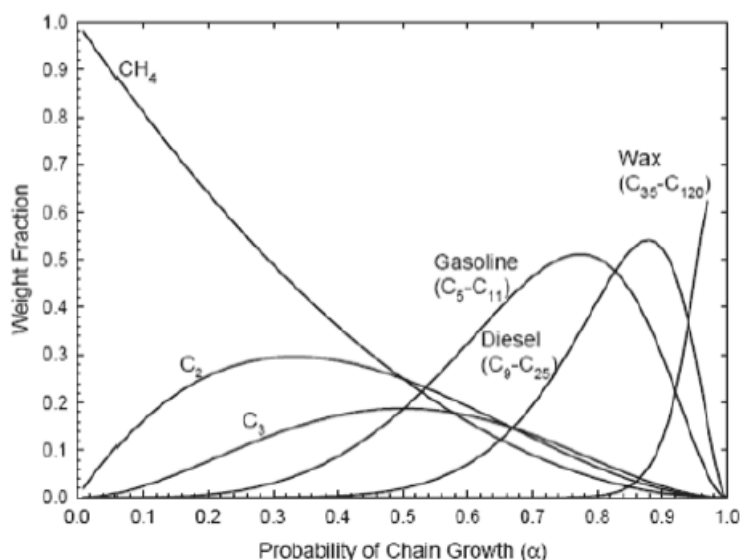


Figure 2 - ASF distribution

After being synthesized, the liquid outlet was sent to upgrading unit and the gas was cooled down before it entered a three-phase separator. The gas out of the three-phase separator was recycled back to the pre-reformer and FT reactor. There was a purge gas to avoid accumulation of CO_2 , which was inert in the FT synthesis. The purge gas was assumed used as fuel for the fired heaters. Water was removed in the three-phase separator and lighter hydrocarbons were sent to upgrading unit.

The hydrocarbons separated out, were heated to 510-630 K, before they entered a hydrotreater along with hydrogen gas (20). The hydrogen gas was produced in a hydrogen plant.

2.3 Upgrading unit

In the hydrotreater, cracking and isomerization took place, and the wanted products were mainly branched paraffins in the middle distillate ($\text{C}_{10}\text{-C}_{20}$), since these were the most valuable products.

After being hydrotreated, the fluid was fractionated in a distillation column. The different fractions were distilled after their boiling points, so each distillation cut approximately corresponded to a saleable fuel. There were 5 cuts in the column; they roughly corresponded to LPG, naphtha, kerosene, diesel and fuel oil.

3. Modelling

The simulation program used in this simulation was Aspen HYSYS® version 7.2.

The fluid package selected was the Peng-Robinson EOS (Equation Of State), because this EOS should be applicable to calculate all fluid properties of natural gas processes (21).

Along with the simulation program, a modelling program called MATLAB (MATrix LABoratory) was used. This program is based on the script language C, and is one of the most used mathematical programs for engineers.

3.1 Combining HYSYS and MATLAB

To get MATLAB and HYSYS to cooperate, MATLAB was used to create an interface between the two programs via an ActiveX server. This server allowed MATLAB to get values from HYSYS, and send values back. A possible routine for doing this is shown below in Table 4.

Table 4 - Routine for opening an ActiveX server (22)

<code>h=actxserver('HYSYS.Application')</code>	Creates an ActiveX server
<code>hyCase=h.Activedocument</code>	Call the active simulation
<code>Sol=hyCase.Solver</code>	Call the HYSYS solver
<code>f=hyCase.Flowsheet</code>	Call the current flowsheet
<code>g=f.Materialstreams</code>	Call a material stream
<code>Sol.CanSolve=1</code>	Turn on the HYSYS solver

To get a value from HYSYS the code `a="g.Item ('X').Y"` was used. Where X was replaced by the name of the stream, Y was replaced by the wanted value i.e. TemperatureValue, PressureValue, MassFlowValue etc. and a was the name of the variable in MATLAB.

For sending a value back to HYSYS the opposite was done. `"g.Item(X).Y=a"`

3.2 Modelling in HYSYS

The fired heaters seen on Figure 1 were modeled as heaters, and heat exchangers were modeled as heaters or coolers, this was done to simplify the simulations.

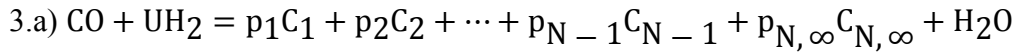
The pre-reformer was modeled as an equilibrium reactor. Reaction 2.a is actually a conversion reaction, but since the temperature inside the reactor was high, all higher hydrocarbons were completely converted, so it was ok to use an equilibrium reactor. The temperature in the pre-

reformer was set to 455 °C, because that temperature was large enough to give an ethane conversion of 99,999 %. If the temperature was higher, the ethane conversion would have been slightly higher, but the fired heater and pre-reformer would be more expensive.

The ATR was modeled as an equilibrium reactor. This assumption was made because the outlet temperature was so high (1030 °C) that equilibrium was a good assumption. The temperature into the ATR was set to 650 °C. This temperature could have been lower, but then the ASU would have been more expensive. The temperature should not exceed 675 °C due to limitations on construction material (18), (23).

The pressure drops in heat exchangers were set to 35 kPa for liquids and 1 bar for gases (24).

The Fischer-Tropsch reactor was modeled as a continuous stirred tank reactor (CSTR), and the reaction was heterogeneous catalytic. The actual FT-reactor was a slurry bubble column reactor. A CSTR model was used because the reaction was in liquid phase, and the liquid phase in a slurry bubble column can be approached as an ideal CSTR. The overall FT reaction was modeled as one reaction, and written as



Since the database in HYSYS only contained hydrocarbons up to C_{30} , a remainder distribution was defined based on the average carbon number for hydrocarbons above C_{20} (25).

$$x_{[N,\infty]} = N + \frac{\alpha}{1-\alpha} = 30 \quad (3.1)$$

$$\text{This means that } C_{[N,\infty]} = C_{30} \text{ represented } \sum_{N=21}^{\infty} C_N \quad (3.2)$$

The U and p_i values were calculated in Appendix D, α was 0.9 and N was 21.

The pressure drop in the reactor was neglected, because it was a slurry bubble column, and therefore the pressure drop would be low. The pressure drops in the heat exchangers were large, so they compensated for the neglected pressure drop in the reactor.

There was assumed only formation of paraffins in the FT synthesis, olefin and alcohol formation were neglected.

The distillation column was modeled as shortcut columns. This was done to simplify the simulations, because a distillation column was harder to converge.

3.3 Reactor Model for hydrotreater

The most common reactor used for hydrotreating is a trickle bed reactor which entails movement of both liquid and gas over a catalyst bed. Using a trickle bed reactor implies that there is no catalyst abrasion, and that a plug flow model can be applied (26). The proposed model used in the simulation was a plug flow model (PFM) as suggested by Pellegrini (12).

To solve the equations, MATLAB was used. The iteration routine used in MATLAB is called ode45, which can solve nonstiff ordinary differential equations.

For MATLAB to solve the equations it was important that all equations were on the form given in equation 3.3.

$$\frac{d\Psi_i}{dV} = f(\Psi_i) \quad (3.3)$$

Where Ψ can be mass fractions (ω), temperature (T) or total pressure (P)

In addition to the equations, boundary and initial conditions were needed. Since this was a first order differential problem in only one variable, one boundary condition was needed for each equation. The boundary conditions used were at the inlet of the reactor, and were sent to MATLAB from the simulation in HYSYS. The boundary conditions were on the form given in equation 3.4.

$$\Psi(V=0) = \Psi_0 \quad (3.4)$$

In the model it was assumed that all reaction happened in vapor phase. Further it was assumed that the superficial gas velocity and the viscosity were constant throughout the reactor.

3.3.1 General equations

The general equations for conservation of mass and energy are (27);

Conservation of mass

$$\frac{\partial}{\partial t}(\rho\omega_s) + \nabla \cdot (\rho\mathbf{v}\omega_s) = -\nabla \cdot \underline{j_s} + R_s \quad (3.5)$$

Conservation of energy

$$\rho C_{p, mass} \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = -\nabla \cdot \underline{q} - \frac{T}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_{p, \omega} \frac{Dp}{DT} - \sigma : \nabla \underline{v} + \sum_{s=1}^n \frac{\bar{h}_s}{M_s} \nabla \cdot \underline{j}_s + \sum_{r=1}^Q \frac{R_r}{M_{A_{ref}}} (-\Delta H_{rx, r}) \quad (3.6)$$

For the hydrotreater where a PFM was applied, these equations could be simplified to

Conservation of mass

$$\frac{d\omega_s}{dV} = \frac{M_s}{\dot{m}} \sum_j \nu_{ij} r_j \quad (3.7)$$

Conservation of energy

$$\frac{dT}{dV} = \frac{\tilde{M}}{\dot{m} \tilde{C}_{p, molar}} \sum_{r=1}^Q r_r (-\Delta H_{rx, r}) \quad (3.8)$$

A complete view of the derivation and simplifications of the equations can be found in Appendix C.

3.3.2 Lumped kinetics

In this project a lumped kinetic model was chosen. There were nine different lumps used, n-C₁₋₄, n-C₅₋₉, n-C₁₀₋₁₄, n-C₁₅₋₂₀, n-C₂₁, iso-C₅₋₉, iso-C₁₀₋₁₄, iso-C₁₅₋₂₀, iso-C₂₁₊.

The lumped kinetic model gives a less accurate system (12), but the computational time needed is less, and the number of parameters needed is less compared to other models.

The lumped kinetics model chosen is able to represent the yields of different lumps with sufficiently high accuracy as well as it takes the variability of different factors into account, such as temperature and pressure (12).

As an alternative to the lumped kinetic model, several models based on the “single event” have been applied in other projects (28), (29). The problems with single event models are their limitations to only a few components, due to the lack of kinetic parameters for all possible isomers.

A third option is the “all component hydrocracking model” described by Pellegrini (30) and Fernandes (20). These models calculate estimates for the kinetic parameters based on the number of carbon atoms in the compound.

In this project an additional lumping occurred when the results from MATLAB were sent back to HYSYS. The HYSYS databank contained iso-compounds only up to C₁₀, so the lumps i-C₁₀₋₁₄, i-C₁₅₋₂₀ and i-C₂₁₊ were lumped into a new lump called i-C₁₀₊. Because of this lump the product streams named ‘Kerosene’, ‘Diesel’ and ‘Fuel oil’ in the flowsheet were one stream in HYSYS, which was named ‘Fuel oil/diesel/kerosene’. The fractions of fuel oil, diesel and kerosene in that stream were calculated from MATLAB.

3.3.3 Complete reactor model

This chapter will show the main equations used for solving the hydrotreater.

3.3.3.1 Species mass balance

The rate expressions for cracking and isomerization are (12);

$$r_{iso} = \frac{k_{iso} \left(p_{n-c} - \frac{p_{iso-c}}{K_{eq}} \right) - k_{cr} p_{iso-c}}{ADSORB} \quad (3.9)$$

$$r_{cr} = \frac{k_{cr} p_{iso-c}}{ADSORB} \quad (3.10)$$

Where

$$ADSORB = p_{H_2} \left[1 + \sum_i K_{L_{n-c,i}} p_{n-c,i} + K_{L_{iso-c,i}} p_{iso-c,i} \right] \quad (3.11)$$

$$k_{cr} = \rho_{cat} k_{cr}^0 \exp \left[\frac{-E_{cr}}{RT} \right] \quad (3.12)$$

and

$$k_{iso} = \rho_{cat} k_{iso}^0 \exp \left[\frac{-E_{iso}}{RT} \right] \quad (3.13)$$

The reaction network in Figure 3 shows which reactions were present, and whether they were irreversible or reversible.

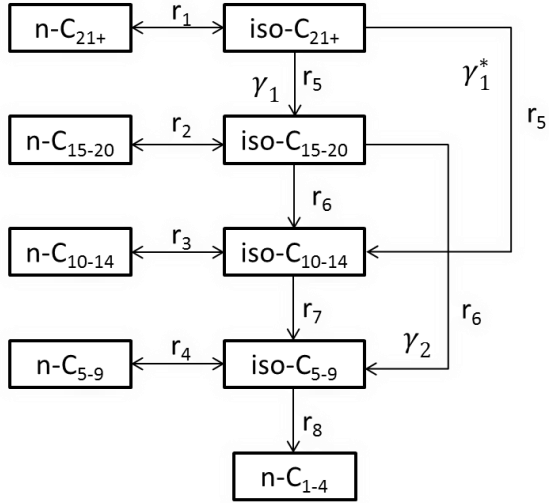


Figure 3 - Reaction network

The expressions used for the reaction rates are given below

$$r_1 = \frac{k_{iso,21+} \left(p_{n,21+} - \frac{p_{i,21+}}{K_{eq,21+}} \right)}{ADSORB} \quad (3.14)$$

$$r_2 = \frac{k_{iso,15-20} \left(p_{n,15-20} - \frac{p_{i,15-20}}{K_{eq,15-20}} \right)}{ADSORB} \quad (3.15)$$

$$r_3 = \frac{k_{iso,14-10} \left(p_{n,14-10} - \frac{p_{i,14-10}}{K_{eq,14-10}} \right)}{ADSORB} \quad (3.16)$$

$$r_4 = \frac{k_{iso,5-9} \left(p_{n,5-9} - \frac{p_{i,5-9}}{K_{eq,5-9}} \right)}{ADSORB} \quad (3.17)$$

$$r_5 = \frac{k_{iso,21+} p_{iso,21+}}{ADSORB} \quad (3.18)$$

$$r_6 = \frac{k_{iso,15-20} p_{iso,15-20}}{ADSORB} \quad (3.19)$$

$$r_7 = \frac{k_{iso,10-14} p_{iso,10-14}}{ADSORB} \quad (3.20)$$

$$r_8 = \frac{k_{iso,5-9} p_{iso,5-9}}{ADSORB} \quad (3.21)$$

The reaction rate expressions for the different lumps will then be;

$$r_{n-C_{1-4}} = 2r_8 \quad (3.22)$$

$$r_{n-C_{5-9}} = -r_4 \quad (3.23)$$

$$r_{n-C_{10-14}} = -r_3 \quad (3.24)$$

$$r_{n-C_{15-20}} = -r_2 \quad (3.25)$$

$$r_{n-C_{21+}} = -r_1 \quad (3.26)$$

$$r_{iso-C_{5-9}} = r_4 + 2r_7 + 2\gamma_2 r_6 - r_8 \quad (3.27)$$

$$r_{iso-C_{10-14}} = r_3 + 2(1-\gamma_2)r_6 + 2\gamma_1^* r_5 - r_7 \quad (3.28)$$

$$r_{iso-C_{15-20}} = r_2 + 2\gamma_1 r_5 - r_6 \quad (3.29)$$

$$r_{iso-C_{21+}} = r_1 - (\gamma_1 + \gamma_1^*) r_5 \quad (3.30)$$

There were two different sets of parameters tested, and they are both given in Table 9 in Chapter 3.5. The gammas represented how much of the old lump which was cracked into the new lump, and they were fitted to give results approximately like the ones in Pellegrini (12). The values used in Pellegrini (12) were not used, because the last lump was not equal. In this project the last lump represented all hydrocarbons which had a carbon number equal to or higher than 21, while in Pellegrini (12) the last lump represents hydrocarbons with a carbon number higher than 22. γ_1 , γ_1^* and γ_2 were set to 1/2, 1/3 and 9/16.

The complete model for the species mass balance was

$$\frac{d\omega_{n-C_{1-4}}}{dV} = \frac{M_{n-C_{1-4}}}{\dot{m}} \cdot r_{n-C_{1-4}} \quad (3.31)$$

$$\frac{d\omega_{n-C_{5-9}}}{dV} = \frac{M_{n-C_{5-9}}}{\dot{m}} \cdot r_{n-C_{5-9}} \quad (3.32)$$

$$\frac{d\omega_{n-C_{10-14}}}{dV} = \frac{M_{n-C_{10-14}}}{\dot{m}} \cdot r_{n-C_{10-14}} \quad (3.33)$$

$$\frac{d\omega_{n-C_{15-20}}}{dV} = \frac{M_{n-C_{15-20}}}{\dot{m}} \cdot r_{n-C_{15-20}} \quad (3.34)$$

$$\frac{d\omega_{n-C_{21+}}}{dV} = \frac{M_{n-C_{21+}}}{\dot{m}} \cdot r_{n-C_{21+}} \quad (3.35)$$

$$\frac{d\omega_{iso-C_{5-9}}}{dV} = \frac{M_{iso-C_{5-9}}}{\dot{m}} \cdot r_{iso-C_{5-9}} \quad (3.36)$$

$$\frac{d\omega_{iso-C_{10-14}}}{dV} = \frac{M_{iso-C_{10-14}}}{\dot{m}} \cdot r_{iso-C_{10-14}} \quad (3.37)$$

$$\frac{d\omega_{iso-C_{15-20}}}{dV} = \frac{M_{iso-C_{15-20}}}{\dot{m}} \cdot r_{iso-C_{15-20}} \quad (3.38)$$

$$\frac{d\omega_{iso-C_{21+}}}{dV} = \frac{M_{iso-C_{21+}}}{\dot{m}} \cdot r_{iso-C_{21+}} \quad (3.39)$$

$$\frac{d\omega_{H_2}}{dV} = \sum_{i=1}^9 \frac{d\omega_{C_{si}}}{dV} \quad (3.40)$$

3.3.3.2 Relationship between mass fractions and partial pressures

To transform equation 3.9 and 3.10 to the form in equations 3.31-3.40, a relationship between partial pressures and mass fractions had to be derived.

The basis for this relationship was Dalton's law, which relates the partial pressures and mole fractions.

$$p_i = y_i P \quad (3.41)$$

The mole fractions can be converted to mass fractions according to equation 3.42.

$$y_i = \omega_i \frac{M_{mix}}{M_i} \quad (3.42)$$

Where M_{mix} is the molar mass of the mixture, and is expressed as

$$M_{mix} = \frac{1}{\sum_{i=1}^N \frac{\omega_i}{M_i}} \quad (3.43)$$

3.3.3.3 Temperature equation

The temperature equation used is given in equation 3.8

$$\frac{dT}{dV} = \frac{\tilde{M}}{\dot{m}\tilde{C}_{p,molar}} \sum_{r=1}^Q r_r (-\Delta H_{rx,r}) \quad (3.8)$$

The different parameters needed to calculate the temperature profile are given in Table 5.

Table 5 - Parameters used in energy equation

Lump	Compound used	Cp $\left[\frac{kJ}{kgmole} \right]$	Cp reference	ΔH_{298}^0 $\left[\frac{kJ}{kgmole K} \right]$	ΔH_{298}^0 reference
n-C ₁₋₄	Mean value	65	(31)	-97429.5	(32)
n-C ₅₋₉	Mean value	166	(31)	-187890	(32)
n-C ₁₀₋₁₄	Mean value (ΔH), dodecane (Cp)	280	(31)	-291070	(32)
n-C ₁₅₋₂₀	Mean value (ΔH), octadecane (Cp)	515.8	(32)	-404503	(32)
n-C ₂₁₊	n-C ₃₀	960.4	(32)	-664200	(32)
iso-C ₅₋₉	3-methylhexane	210.9	(32)	-192390	(32)
iso-C ₁₀₋₁₄	5-methylundecane	372	(33)	-295200	(33)
iso-C ₁₅₋₂₀	2-methylheptadecane	536	(33)	-419700	(33)
iso-C ₂₁₊	2,6,10,15,19,23- hexamethyltetracosane (squalane)	886.36	(34)	-864700	(35)
H ₂	H ₂	29	(31)	0	(32)
H ₂ O	H ₂ O	34	(31)	-241814	(32)
CO	CO	29	(31)	-110590	(32)
CO ₂	CO ₂	37	(31)	-393790	(32)

The molecular structures of the iso-compound used to represent the different lumps are drawn in Figure 4.

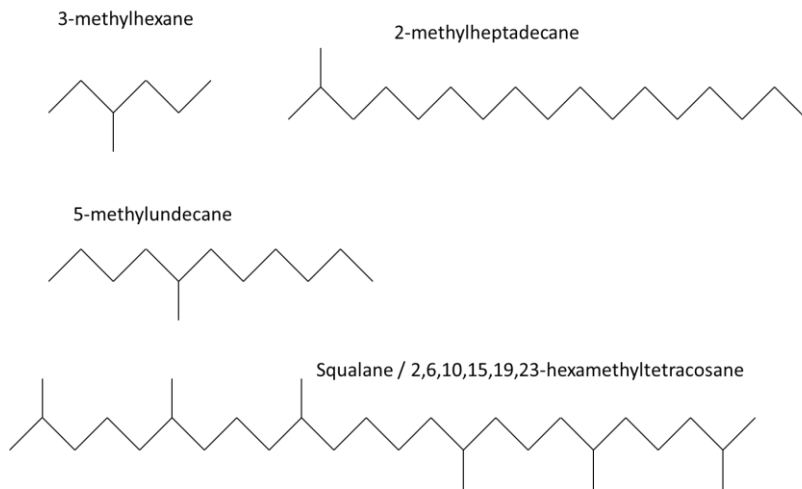


Figure 4 - Molecular structures of iso-compounds

3.3.3.4 Pressure loss

To calculate the pressure loss, Ergun's equation was used (36). This equation can be used to calculate pressure drops across fixed catalyst beds.

$$\frac{dP}{dz} = -f \frac{\rho_f (v^s)^2}{d_p} \quad (3.44)$$

Or on volume basis

$$\frac{dP}{dV} = -f \frac{\rho_f (v^s)^2}{Ad_p} \quad (3.45)$$

The friction factor, f , was calculated by the following parameterization proposed by Ergun (36)

$$f = \frac{1-\varepsilon}{\varepsilon^3} \left[1.75 + \frac{150(1-\varepsilon)}{\text{Re}_{p}} \right] \quad (3.46)$$

The Reynolds number was calculated according to equation 3.47

$$\text{Re}_{p} = \frac{v^s d_p \rho_f}{\mu_f} \quad (3.47)$$

The different parameters used to calculate the pressure drop in the hydrotreater are given in Table 6.

Table 6 - Parameters used to calculate pressure loss

Parameter	Meaning	Unit	Value	Reference
μ	Viscosity	cP	0.02535	HYSYS
ε	Void fraction	$\frac{m_{catalyst}^3}{m_{reactor}^3}$	0.8	(20)
d_p	Particle diameter	m	$3 \cdot 10^{-3}$	(37)
v^s	Superficial gas velocity	m/s	0.5336	Calculated

The superficial gas velocity was calculated from the volumetric gas flow according to equation 3.48.

$$v^s = \frac{V_g^*}{A} \quad (3.48)$$

3.4 Total Mass and Energy balances

When using a simulation tool like HYSYS it was important to check the overall mass and energy balances to make sure they were conserved.

3.4.1 Total mass balance

The general mass equation at steady state is given in equation 3.49

$$\sum m_{In}^* = \sum m_{Out}^* \quad (3.49)$$

The values gotten from HYSYS are given in Table 7.

Table 7 - Total mass balance

Inlet Streams	m* [kg/h]	Outlet Streams	m* [kg/h]
Natural gas	143 368	Water out 1	127 532
Steam	126 106	Water out 2	158 747
Oxygen in	167 902	Purge	42 995
Hydrogen in	7 500	Naphtha	22 707
		Naphtha 2	901
		Fuel oil/diesel/kerosene	91 980
Sum	444 875	Sum	444 862
In-out	13		
% wrong of inlet stream	0.003		

There was a slight error in the total mass balance, and it was associated with the recycle loops in HYSYS which all contained a small error.

3.4.2 Total energy balance

The general energy equation for a steady state process is given below

$$\sum Q_{in} = \sum Q_{InletStreams} + \sum Q_{Added} = \sum Q_{OutletStreams} + \sum Q_{removed} = \sum Q_{out} \quad (3.50)$$

The values gotten from HYSYS are given in Table 8.

Table 8 - Total energy balance

Inlet Streams	Q [kW]	Outlet Streams	Q [kW]
Natural gas	-174 569	Water out 1	-561 559
Steam	-441 170	Water out 2	-694 606
Oxygen in	7 518	Purge	-95 289
Hydrogen in	-2	Naphtha	-10 223
Duty1	60 497	Naphtha 2	-406
		Fuel	
Duty2	51 686	oil/diesel/kerosene	-27 611
Duty4	115 195	DutyFT	-393 523
Duty6	1 945	Duty3	425 161
Duty7	171	Duty5	208 789
Duty8	33 656	Duty10	-1 696
Duty9	-4 118	Duty11	-4 118
Duty12	175	Duty13	-4 118
Duty14	10 247		
Sum	-338 768	Sum	-352 289
In-out	13 521		

The total energy balance was not conserved in HYSYS. This was expected and was due to the lumping of components from MATLAB to HYSYS as mentioned in Chapter 3.3.2. Since all higher iso-components than 10 were lumped in one, information regarding heat flow was lost.

3.5 Two sets of parameters

There were two different sets of kinetic parameters tested. Model 1 (12) and Model 2 (30). Model 1 gave parameters for the lumped kinetics model, while Model 2 gave parameters for the “all component model”, but the parameters could still be used for a lumped model, since they were assumed constant over a given interval. The main difference between them was the magnitude of the rate constants for cracking. The parameters for the two models are compared in Table 9 below.

Table 9 - Parameters for the two models

Lump	K_{eq}	k_{iso}^0 $\left[\frac{kmol}{kg\ h} \right]$	k_{cr}^0 $\left[\frac{kmol}{kg\ h} \right]$	$K_{L_{iso}}^0$ [Pa ⁻¹]	$K_{L_{cr}}^0$ [Pa ⁻¹]	E_{iso} $\left[\frac{kJ}{kmol} \right]$	E_{cr} $\left[\frac{kJ}{kmol} \right]$
Model 1							
C ₁₋₄	-	-	-	-	$5.46 \cdot 10^{-2}$	-	-
C ₅₋₉	$7.19 \cdot 10^2$	$1.14 \cdot 10^{23}$	$4.48 \cdot 10^{22}$	5.46	5.47	$1.94 \cdot 10^5$	$1.30 \cdot 10^5$
C ₁₀₋₁₄	$8.36 \cdot 10^2$	$2.60 \cdot 10^{24}$	$9.50 \cdot 10^{24}$	54.8	54.8	$1.94 \cdot 10^5$	$1.66 \cdot 10^5$
C ₁₅₋₂₀	$3.76 \cdot 10^3$	$9.47 \cdot 10^{27}$	$7.05 \cdot 10^{26}$	946	$9.05 \cdot 10^2$	$1.94 \cdot 10^5$	$1.82 \cdot 10^5$
C ₂₁₊	$5.73 \cdot 10^3$	$2.80 \cdot 10^{29}$	$7.90 \cdot 10^{27}$	$9.53 \cdot 10^7$	$7.19 \cdot 10^7$	$2.06 \cdot 10^5$	$1.87 \cdot 10^5$
Model 2							
C ₁₋₄	-	-	-	-	$5.46 \cdot 10^{-2}$	-	-
C ₅₋₉	$3.59 \cdot 10^3$	$1.14 \cdot 10^{23}$	$4.48 \cdot 10^{22}$	5.46	5.47	$1.61 \cdot 10^5$	$1.34 \cdot 10^5$
C ₁₀₋₁₄	$3.78 \cdot 10^3$	$7.60 \cdot 10^{24}$	$4.50 \cdot 10^{24}$	54.8	54.8	$1.68 \cdot 10^5$	$1.65 \cdot 10^5$
C ₁₅₋₂₀	$3.86 \cdot 10^3$	$9.47 \cdot 10^{27}$	$3.05 \cdot 10^{26}$	946	$9.05 \cdot 10^2$	$1.92 \cdot 10^5$	$1.85 \cdot 10^5$
C ₂₁₊	$5.93 \cdot 10^3$	$2.80 \cdot 10^{29}$	$2.99 \cdot 10^{27}$	$9.53 \cdot 10^7$	$7.19 \cdot 10^7$	$2.01 \cdot 10^5$	$1.93 \cdot 10^5$

The plots for the mass fraction profiles of hydrocarbons and the temperature profiles can be seen on the next pages.

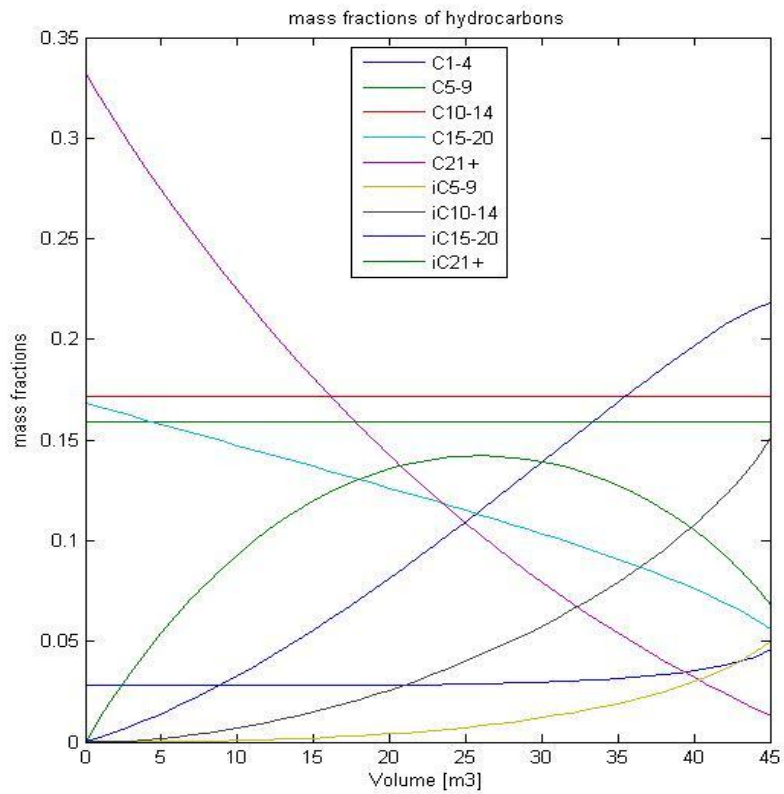


Figure 5 - Mass fractions Model 1

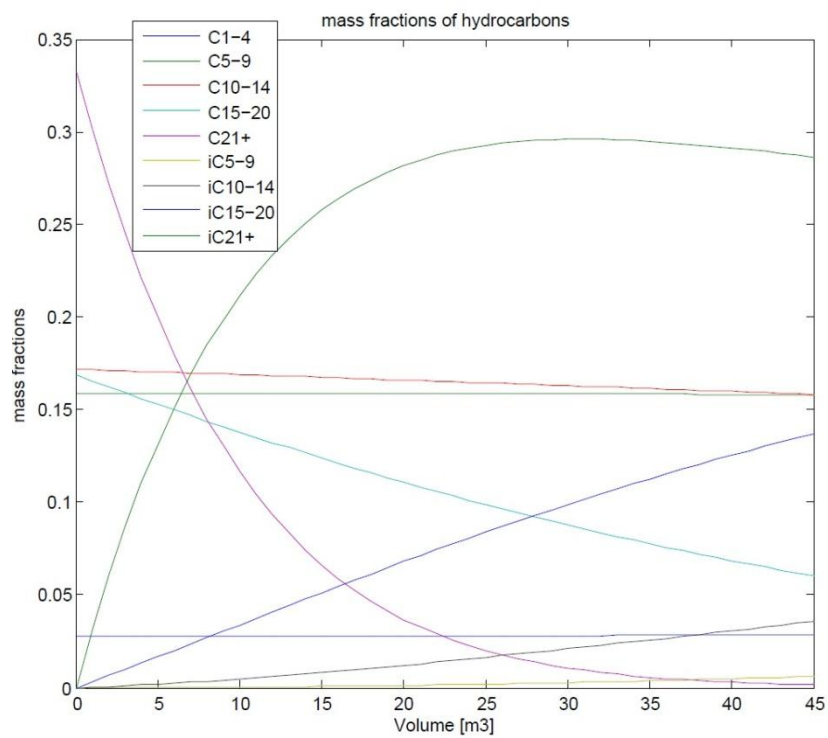


Figure 6 - Mass fractions Model 2

For a given reactor volume, H_2 /wax ratio, temperature and pressure, Model 1 estimated faster cracking reactions than Model 2. This can be seen by the mass fractions of the lump iC_{21+} which are much higher in Figure 6, whilst Model 1 predicted that a large fraction of that lump had been cracked into smaller fractions (iC_{15-20} and iC_{10-14}) as seen in Figure 5. Cracking reactions are slower than isomerization reactions (38), so both models fit the predictions.

The temperature plots for the two models had some differences, as shown in Figure 7 and Figure 8.

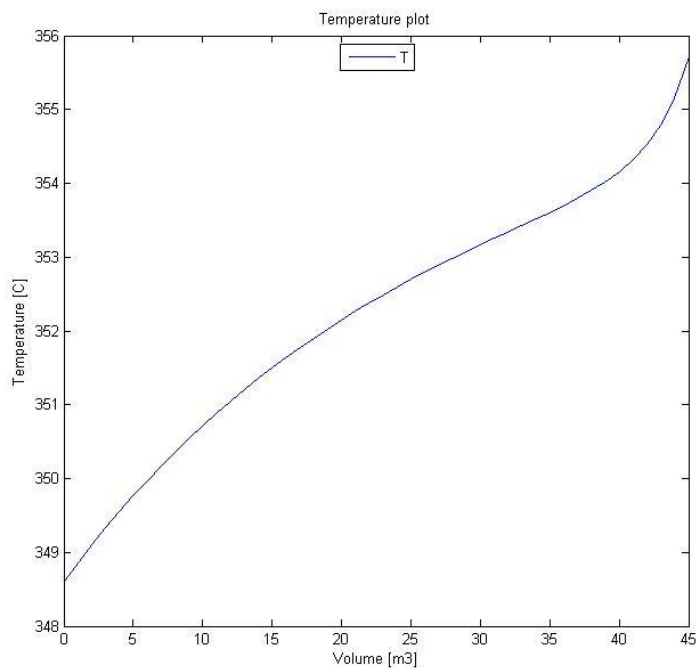


Figure 7 - Temperature plot Model 1

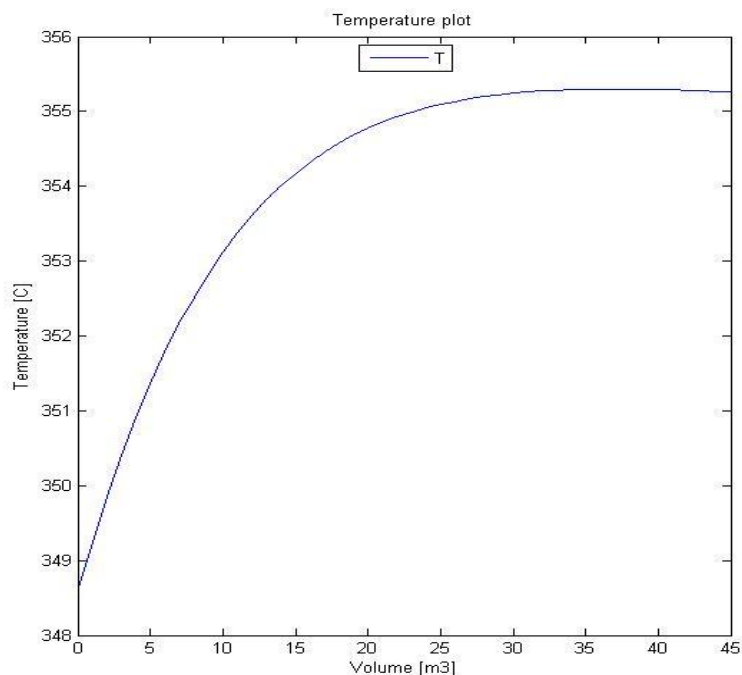


Figure 8 - Temperature plot Model 2

Isomerization reactions are mildly exothermic, and an increase in temperature was expected, which both models showed. The difference was the cracking reaction, which is more exothermic than the isomerization reactions (38). Model 1 predicted this well, as the slope changes significantly, whilst Model 2 predicted a temperature drop when cracking started. This prediction does not fit with the theory, and can only be right if the isomerization reactions were reversed at this point, but as seen from Figure 6 this was not the case. Only Model 1 showed the predicted results for the temperature profile inside the reactor.

The pressure drops inside the reactor were pretty similar for both models, and are not shown. On behalf of this information Model 1 was chosen in the further work because it was the model used for lumped kinetics model and also predicted the most predicted temperature profile compared to literature.

4. Optimization and Results

This chapter shows the optimization and results for the hydrotreater. The MATLAB script used for these results can be found in Appendix D. In addition the MATLAB and HYSYS files are given as electronic appendices in Appendix F.

4.1 Hydrotreater

A typical industrial reactor for hydrotreating is about 30-35 m³ (39). The catalyst assumed used was consisted of platinum (0.6%) supported on amorphous silica alumina extruded with a γ -alumina binder (12). The bulk density of the catalyst was 950 kg/m³, and the porosity 0.80 (20). The cost of these catalysts ranged from 9-12 \$/lb (40). The diameter of the catalyst particles were in the area of 1.5-3 mm (37).

4.2 Optimization of hydrotreater

The optimal conditions for the hydrotreater were considered from an economic point of view, which means that the values found were not necessarily the values that gave highest production of fuels, but they gave highest profitability of the plant. The profitability was measured in net present value (NPV), internal rate of return (IRR) and return on investment (ROI). The net present value is found from equation 4.1 where CF is cash flow in year j, i is the discount rate and I₀ is the investment cost. The internal rate of return (IRR) is the discount rate (i) that gives NPV=0.

$$NPV = -I_0 + \sum_{j=1}^{lifetime} \frac{(CF)_j}{(1+i)^j} \quad (4.1)$$

The discount rate was set to 9%, and the lifetime was set to 20 years. Taxes were set to 30%, and a reducing balance depreciation of 20% was used.

Another method to measure the efficiency of a project is the return on investment (ROI) which is the ratio of money gained/lost in an investment relative to the invested money. This method does not take time into account like IRR does. An average over whole project time was used here, and the ROI is defined as (41).

$$ROI = \frac{Cumulative\ net\ profit}{Initial\ Investment \cdot plant\ life} \times 100\% \quad (4.2)$$

The optimized design variables were;

- Hydrotreater inlet pressure
- Hydrotreater inlet temperature
- Hydrotreater volume
- H₂/wax ratio at the inlet of hydrotreater
- With or without recycling of 'LPG' stream

4.2.1 Pressure

The outlet mass fractions were not changed when the total pressure was changed, because hydrogen limited the reactions. If the total pressure decreased the reaction rates were faster, and a less reactor volume was needed to make the reactions happen. As seen from equations 3.9-3.11 the reaction rates of hydrocarbons are invers proportional with the partial pressure of hydrogen. Since hydrogen was the component there was most of in the mixture on molar basis, the reaction rates increased with decreasing hydrogen pressure, which decreased with decreasing total pressure, thus it was favorable with low total pressure. The inlet pressure was the pressure the fluid had after being heated by the fired heater (H-102) which was 25 bars. A depressurization was not done, because too low pressure affects the selectivity (20).

4.2.2 Temperature

To find the optimal temperature of the process, an economic optimization was done. The temperature in to the reactor was plotted against the cost. The hydrotreater volume was not held constant here. The outlet distribution was held constant by changing the hydrotreater volume so the income was the same for all cases. The costs used were only the relevant costs for this particular optimization, they don't say anything special; they're just relative to each other. The costs taken into account were the fired heater (H-102) and the hydrotreater (R-104). The optimal temperature was the one where the extra cost of heating the mixture was lowest. If the inlet temperature increased, the investment and operational cost of the fired heater increased, while the cost of the hydrotreater and catalyst decreased and vice versa. The optimal temperature can be found from Figure 9 where the lowest cost is.

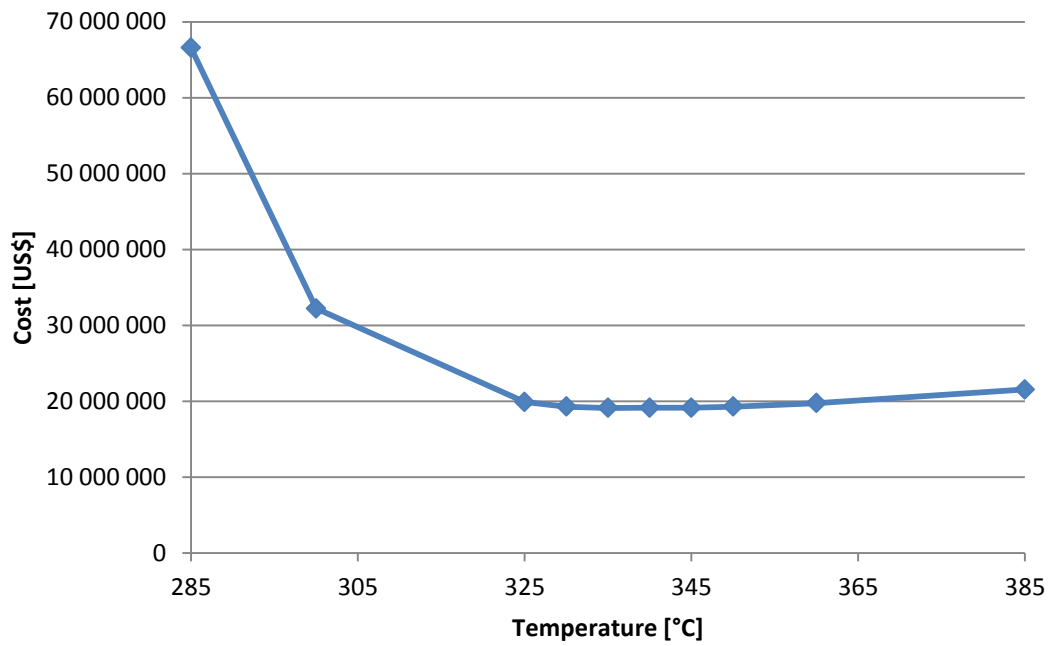


Figure 9 - Temperature vs. cost

As seen from Figure 9, the interval from 325 °C to 365 °C was the optimal temperature interval, and the optimal temperature was 335 °C.

4.2.3 H₂/wax ratio

The H₂/wax ratio is defined as the mass of H₂ divided by the mass of wax going in to the hydrotreater. To calculate the optimal H₂/wax ratio a full economic analysis for the entire plant was done. All economic parameters like natural gas price and product prices were kept constant in all cases. The results can be seen in Figure 10.

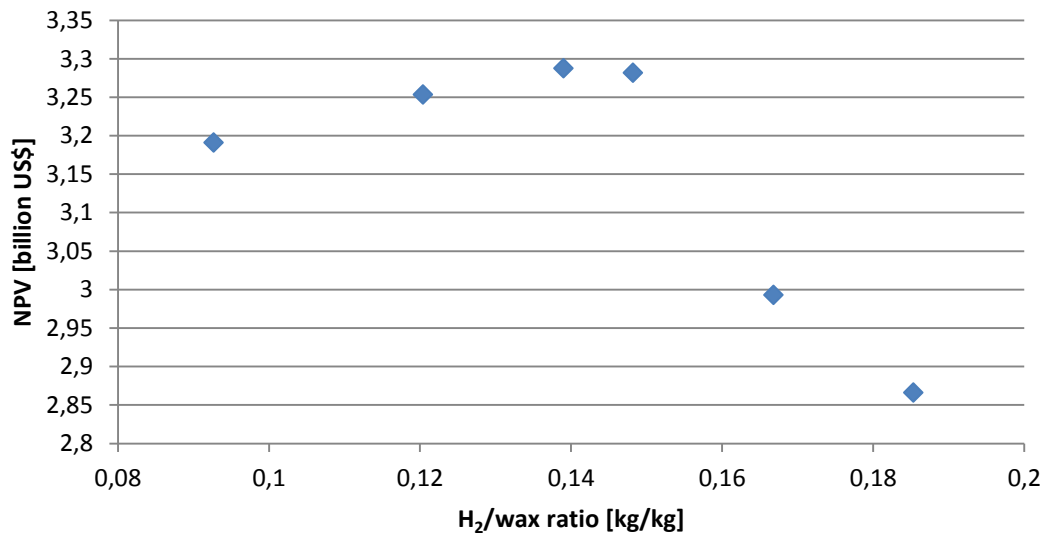


Figure 10 - NPV vs. H₂/wax ratio

The economic optimal H₂/wax ratio was about 0.13-0.14 as seen from Figure 10. If the H₂/wax ratio increased, the profitability went drastically down.

4.2.4 Hydrotreater volume

The hydrotreater volume was minimized with respect to the hydrogen flow. When all the hydrogen was consumed the reactor volume should end, because there would not be any more reactions, and thus there was no point of a larger volume. The only thing gained from a larger volume was larger investment cost, and a higher pressure loss in the reactor. This is illustrated in Figure 11 and Figure 12 on the next page.

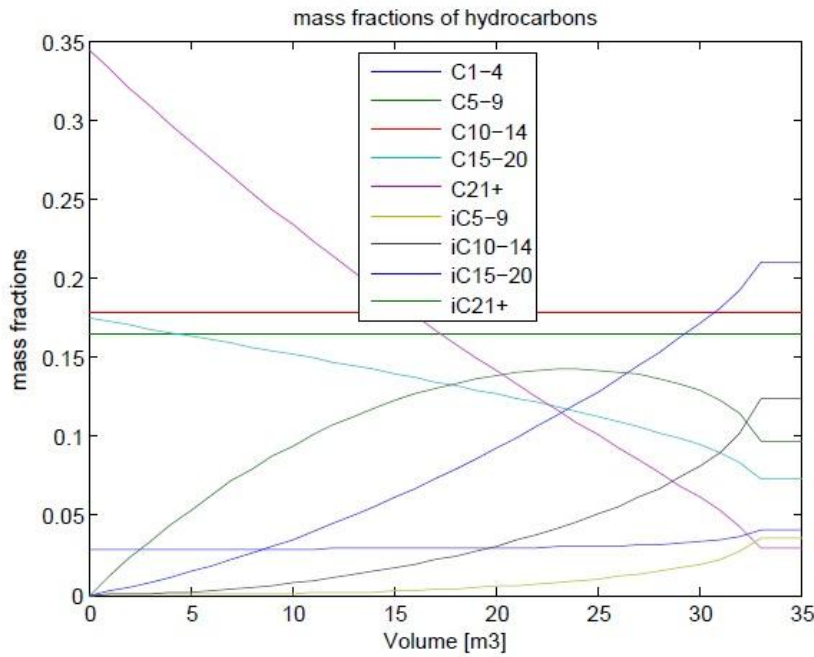


Figure 11 - Too large reactor volume

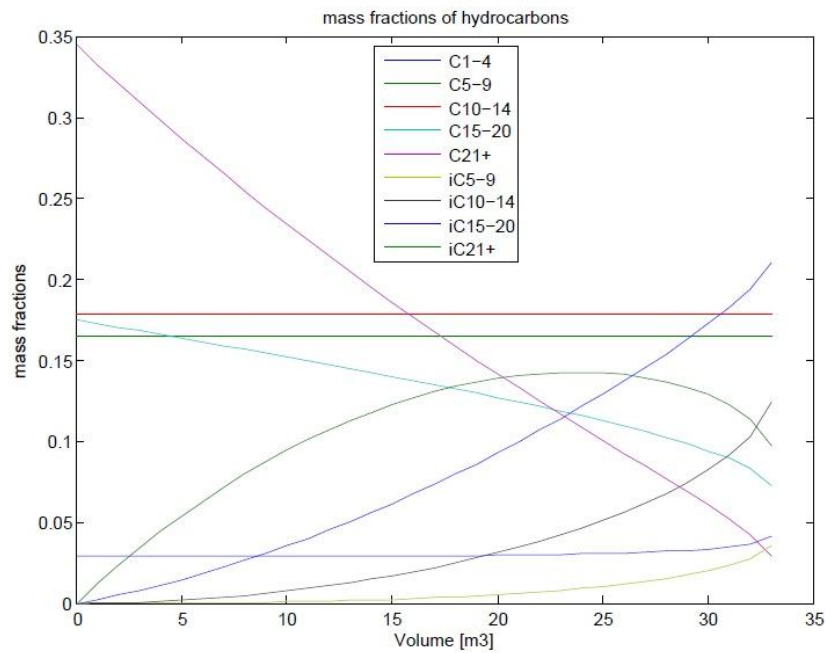


Figure 12 - Perfect reactor volume

As seen from Figure 11, the reactor volume was too large. When the mass fractions flatten all hydrogen was consumed and no further reactions took place after that. In Figure 12 the volume ended when all hydrogen was consumed. The optimal volume was found to be 33 m³.

4.2.5 With/without recycle

There were two different cases tested for the stream named ‘LPG’ in the flowsheets below. One option involved recycling the stream, while the other option was purging the stream.

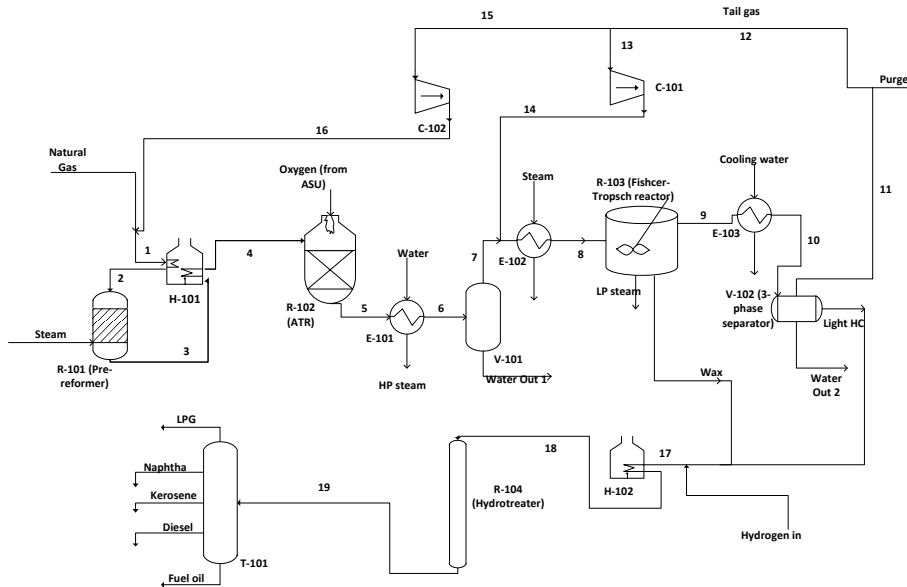


Figure 13 - Flowsheet without LPG recycle

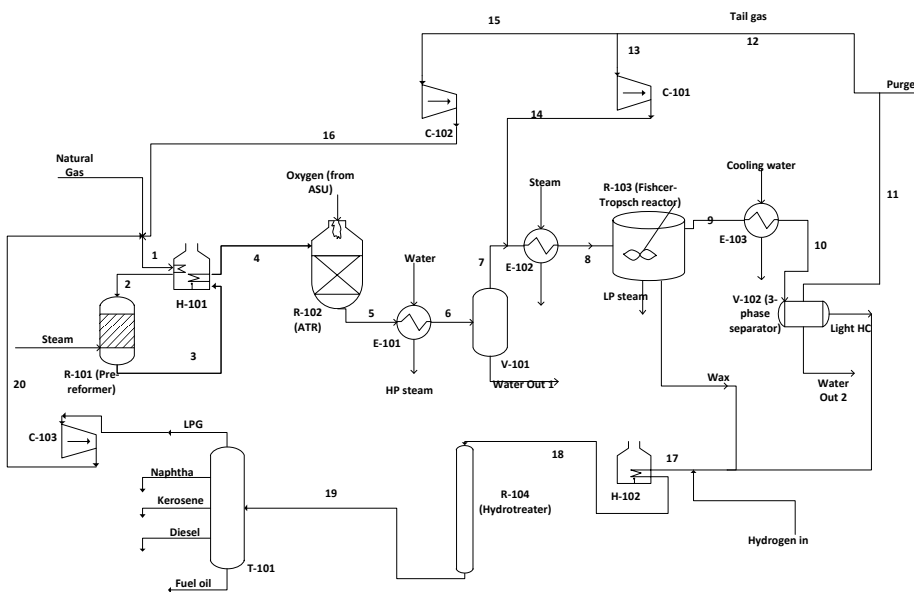


Figure 14 - Flowsheet with LPG recycle

To compare the different cases, the internal rate of return (IRR), net present value (NPV), carbon efficiency and return on investment (ROI) was investigated. The carbon efficiency is defined as

$$\text{Carbon efficiency} = \frac{\text{no. of moles of products} \times \text{no. of carbon atoms in products}}{\text{no. of moles in inlet streams} \times \text{no. of carbon atoms in inlet streams}} \quad (4.3)$$

The key numbers can be found in Table 10. The differences in income, investment costs and production costs can be seen in Figure 15.

Table 10 - Comparison with/without recycle

	With recycle	Without recycle	Difference
Carbon efficiency	89.9 %	85.6 %	4.3 %
Total Production [bbl/day]	23 710	22 600	1 110
Income [million \$/year]	1 105	1 055	50
Fixed capital investment [million \$]	789	759	30
Working capital [million \$]	118	114	4
Total investment cost [million \$]	908	873	35
Production cost [million \$/year]	318	312	6
NPV [million \$]	3 766	3 529	237
IRR	51.9 %	50.8 %	1.1 %
ROI	53%	52%	1%

The net present value, internal rate of return, return on investment and carbon efficiency were all higher when recycling.

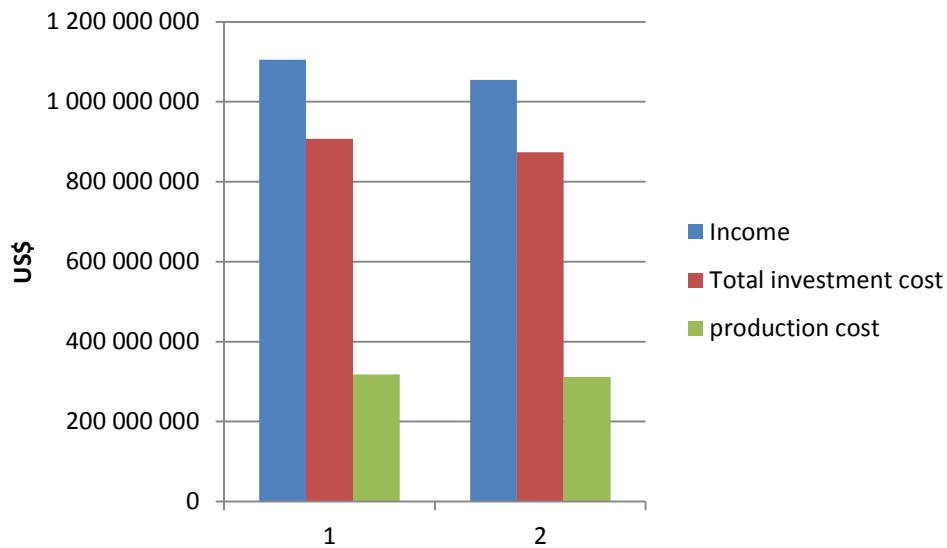


Figure 15 - Comparison with/without recycle

Case 1 represents with recycle and Case 2 without recycle. The income was higher when recycling because the carbon efficiency was higher, and thus the total production of fuels were higher. The total investment cost was higher when recycling, mainly due to an extra compressor needed and a larger air separation unit. The production cost was slightly higher mainly due to higher electricity costs. The alternative chosen in the further work was the case with recycling, since all factors (carbon efficiency, NPV, IRR and ROI) were highest.

4.3 Key factors

The key factors, such as H₂/CO ratio, have not been mentioned so much during this thesis. That is because they were focused on in the earlier report (13). Table 11 summarizes some of the key factors for the entire plant in addition to side streams and products.

Table 11 - Key factors in the plant

Parameter	Value
H ₂ /CO ratio at the inlet of FT reactor [mole/mole]	2.024
Steam/C ratio at the inlet of ATR [mole/mole]	0.5604
Oxygen/C ratio at the inlet of ATR [mole/mole]	0.4789
CO conversion in FT reactor [%]	89.52
H ₂ /wax ratio at the inlet of hydrotreater [kg/kg]	0.133
Carbon Efficiency [%]	89.86
HP Steam used [ton/h]	126.1
Oxygen used [ton/h]	167.9
Hydrogen used [ton/h]	7.5
Naphtha produced [bbl/day]	5 184
Kerosene produced [bbl/day]	7 190
Diesel produced [bbl/day]	7 143
Fuel oil produced [bbl/day]	4 189
Total production [bbl/day]	23 706

The most important properties for the streams in the upgrading unit are given in Table 12 below.

Table 12 - Properties for upgrading unit streams

Stream name	17	18	19	LPG
Temperature [°C]	87	335	344.1	52.4
Pressure [bar]	26	25	25	20
Mass Flow [ton/h]	129	129	129	13
Mass fractions				
ω_{nC1-4}	0.03	0.03	0.04	0.36
ω_{nC5-9}	0.16	0.16	0.16	0.06
ω_{nC10+}	0.70	0.70	0.30	0
ω_{iC5-9}	0	0	0.03	0.02
ω_{iC10+}	0	0	0.41	0
ω_{H2O}	0	0	0	0.01
ω_{H2}	0.06	0.06	0.01	0.07
ω_{CO}	0	0	0	0
ω_{CO2}	0.05	0.05	0.05	0.48
Sum	1.00	1.00	1.00	1.00

5. Economics

This chapter shows how much the different equipment contributed to the total cost.

A summary of which parts contributed most to the total investment cost are given in Table 14. All equipment was assumed made of stainless steel, and stainless steel has a density of 8000 kg/m³ (41).

5.1 Fixed capital investment

To estimate the cost of equipment, a correlation found in Sinnott was used (41). The correlation is given in equation 5.1 below.

$$C_e = a + bS^n \quad (5.1)$$

Where a and b are cost constants, n is an exponent for that equipment and S is the size parameter. The a, b, S and n values for each equipment can be found in appendix A

The installation cost was found using the formula found in Sinnott (41).

$$C = \sum_{j=1}^n C_{e,j,CS} \left[(1 + f_p)f_m + f_{er} + f_{el} + f_i + f_c + f_s + f_l \right] \quad (5.2)$$

The different f- factors are given in Table 13.

Table 13 - f-factors for estimation of fixed capital cost

Parameter	Estimates	Value
$C_{e,j,CS}$	Cost of equipment in carbon steel	
f_p	Piping	0.8
f_m	Material factor	1.3
f_{er}	Equipment erection	0.3
f_{el}	Electrical	0.2
f_i	Instrumentation and control	0.3
f_c	Civil	0.3
f_s	Structures and buildings	0.2
f_l	Lagging and paint	0.1

At last the prices must be scaled to 2011 prices via the CEPCI (Chemical Engineering's Plant Cost Index), according to equation 5.3

$$C_{2011} = C_J \left(\frac{I_{2011}}{I_J} \right) \quad (5.3)$$

Where I is the CEPCI value and J is the year the price of the equipment is from. The 2011 prices for all major equipment are given in Table 14. The sum of all equipment and installation costs are usually defined as ISBL cost (inside battery limit cost). All equipment was made of stainless steel except the catalysts. For more information regarding sizing and cost of equipment and catalysts, see Appendix A. All values in tables in this chapter are given in million US\$. The values were uncertain so there was no point of giving all decimals. The entire values down to each dollar can be found in Excel files given as electronic appendix in Appendix F.

Table 14 - ISBL Cost

ISBL cost 2011 price	Tag name	Cost [million US\$]	% of ISBL cost
Pump 1	P-101	0.1	0.03 %
Pump 2	P-102	0.1	0.03 %
Compressor 1	C-101	11.6	2.68 %
Compressor 2	C-102	4.8	1.11 %
Compressor 3	C-103	5.7	1.32 %
FT reactor	R-103	27.7	6.39 %
Pre-reformer	R-101	2.5	0.58 %
ATR	R-102	10.6	2.45 %
Water Separator	V-101	1.4	0.33 %
3-phase separator	V-102	2.1	0.48 %
Fired heater 1	H-101	23.5	5.42 %
Heat Exchanger 1	E-101	9.6	2.21 %
Heat Exchanger 2	E-102	0.7	0.16 %
Cooling tubes FT reactor		1.6	0.36 %
Heat Exchanger 3	E-103	5.2	1.20 %
Steam Drum 1		3.6	0.82 %
Steam Drum 2		0.5	0.11 %
ASU		185.7	42.81 %
Catalyst		37.1	8.57 %
Fired heater 2	H-102	9.1	2.10 %
Hydrotreater	R-104	0.8	0.18 %
Distillation column	T-101	5.3	1.22 %
Reboiler (dist. column)		0.3	0.07 %
Condenser (dist. column)		0.2	0.04 %
H ₂ plant		83.9	19.34 %
<u>Total ISBL cost</u>		<u>433.8</u>	<u>100.00 %</u>

The most expensive parts of the plant were the oxygen plant (ASU) and hydrogen plant. These two accounted for over 60% of the ISBL cost.

To find the total fixed capital cost, the outside battery limit (OSBL) costs had to be included. The total fixed capital cost is defined as

$$C_{FC} = C(1+OS)(1+D\&E+X) \quad (5.4)$$

Where C_{FC} is the total fixed capital cost, C is the ISBL cost, OS is off-sites, and has a value of 0.3. $D\&E$ is design and engineering, and has a value of 0.3. X is contingent, and has a value of 0.1 (41). Adding the OSBL costs and working capital, the total investment cost was found as seen in Table 15. The working capital is additional money needed in order to run the plant until the plant starts to earn income. The working capital is returned at the end of the project time. For petrochemical industries the working capital is typically 15% of fixed capital investment (41).

Table 15 - Total Investment Cost

Cost	Million US\$
Total ISBL cost	433.8
Off-sites	130.1
Engineering and design	169.2
Contingent	56.4
Fixed Capital Investment	789.4
Working capital	118.4
Total Investment Cost	907.8

5.2 Production costs

The production costs are the costs which are dependent on production, such as electricity and operators.

The number of operators needed was estimated from Turton (42).

$$N_{OL} = \left(6.29 + 31.7P^2 + 0.23N_{np} \right)^{0.5} \quad (5.5)$$

Where P is the number of processing steps involving handling of particulate solids, and N_{np} is the sum of equipment (including compressors, towers, reactors, heaters and heat exchangers). N_{OL} is the number of operators needed per shift, and there are 4.5 shift positions needed (42). In total there were 103 operators needed.

A summary of the production costs can be found in Table 16.

Table 16 - Production costs

Production parameter		Million US\$/year
Electricity	Power consumption from HYSYS used, 0.06 \$/kWh	67.7
Natural gas	Flow from HYSYS used, 2.3 \$/MMbtu	123.9
Operators	103 operators, 60 000 \$/year	6.2
Supervision	25% of Operating labour	1.5
Direct salary overhead	50% of Operating labor + Supervision	3.9
Maintenance	4% of ISBL cost	17.3
Property taxes and insurance	1.5 % of ISBL cost	6.5
Rent of land	1.5% of Fixed capital cost	11.8
General plant overhead	65% of Operating labour + Supervision + Maintenance + Direct overhead	18.8
Allocated environmental charges	1% of Fixed capital cost	7.9
Running license fees and royalty payments	0.5% of ISBL cost	2.2
Waste disposal	41 \$/1000 m ³	7.3
Process water	0.067 \$/1000 kg	0.5
Operation of H ₂ plant		42.1
Total production cost		317.7

The prices for waste disposal, process water and electricity were found in Turton (42). The natural gas price was found from the US Energy administration information (43). The Price for operating the hydrogen plant was found from the US Department of Energy (44). The rest were found in Sinnott (41).

The biggest contributors to the production costs were the natural gas, electricity and operation of the hydrogen plant. The reason why the hydrogen plant was so expensive to operate was because there was assumed that the hydrogen was made from a natural gas plant (44), so natural gas must be bought, while the oxygen plant was cheaper to operate because air is free.

5.3 Income

The parts that contributed to the total income are given in Table 17. Steam was assumed sold, instead of producing electricity via a steam turbine.

Table 17 - Income

Income	Price	Million US\$/year
Nahpta	127.14 \$/bbl	219.7
Kerosene	137.40 \$/bbl	329.3
Diesel	134.60 \$/bbl	320.5
Fuel oil	117.43 \$/bbl	164.0
Sum Products		1 033.5
HP steam	11 £/ton	14.1
LP steam	8.76 £/ton	57.8
Total Income		1 105.4

The steam prices (HP equals high pressure and LP equals low pressure) were found in Sinnott (41), and the product prices were found from OPEC (45). As seen from Table 17, diesel and kerosene were the most valuable fuels.

5.4 Profitability

The profitability was measured in net present value (NPV), internal rate of return (IRR) and return on investment (ROI). The formulas are given in equations 4.1 and 4.2.

$$NPV = -I_0 + \sum_{j=1}^{lifetime} \frac{(CF)_j}{(1+i)^j} \quad (4.1)$$

$$ROI = \frac{Cumulative\ net\ profit}{Initial\ Investment \cdot plant\ life} \times 100\% \quad (4.2)$$

The progress in NPV is shown in Figure 16. The values used here were the values given in tables 14-17.

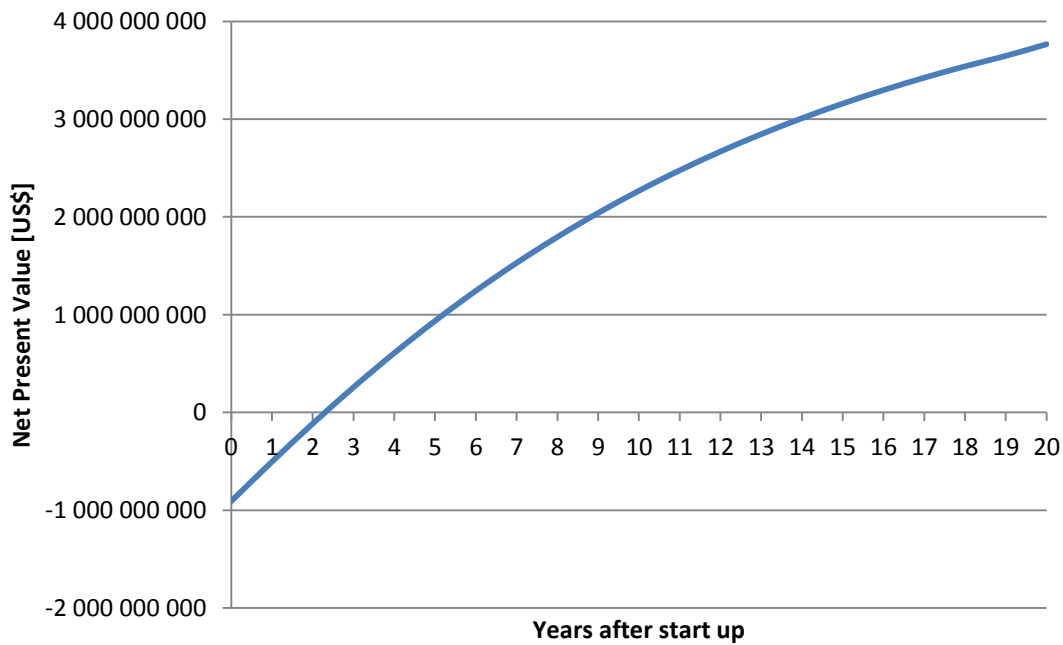


Figure 16 - Net Present Value progress

As seen from the graphic presentation in Figure 16, the project was highly profitable with a discount rate at 9% and 20 years lifetime. The net present value of the project was estimated to 3.8 billion dollars, and an internal rate of return on 52%. The return on investment was 53%.

6. Sensitivity Analysis

A sensitivity analysis was done in order to see how different changes in natural gas price, product prices and tax rate affected the profitability.

6.1 Natural gas price

This chapter will show how the profitability changes with natural gas prices. In all cases the product prices and taxes were held constant. The product prices were the ones given in Table 17 and the tax rate was set to 30%. The change in net present value is given in Figure 17.

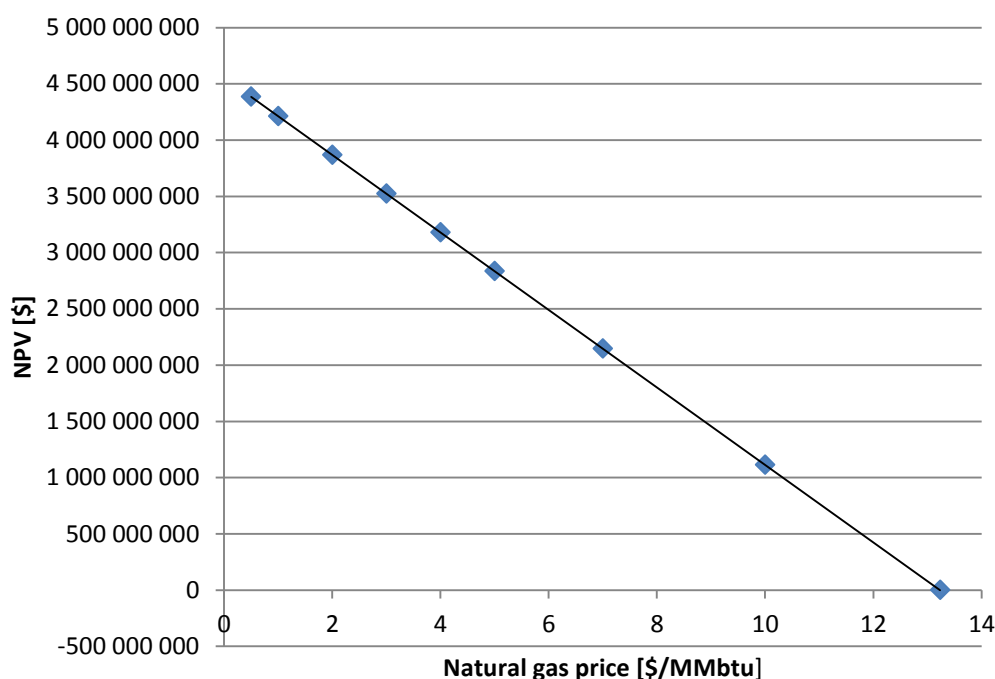


Figure 17 - NPV vs. Natural gas price

As seen from Figure 17, the project is robust against changes in natural gas price. This is due to the high product prices at the time. The project will be profitable up to natural gas prices of 13.235 \$/MMbtu.

6.2 Product prices

The product prices will greatly affect the profitability, and Figure 18 shows how the profitability would have been for different product prices. The natural gas price was 2.3 \$/MMbtu and the tax rate was set to 30% in all cases.

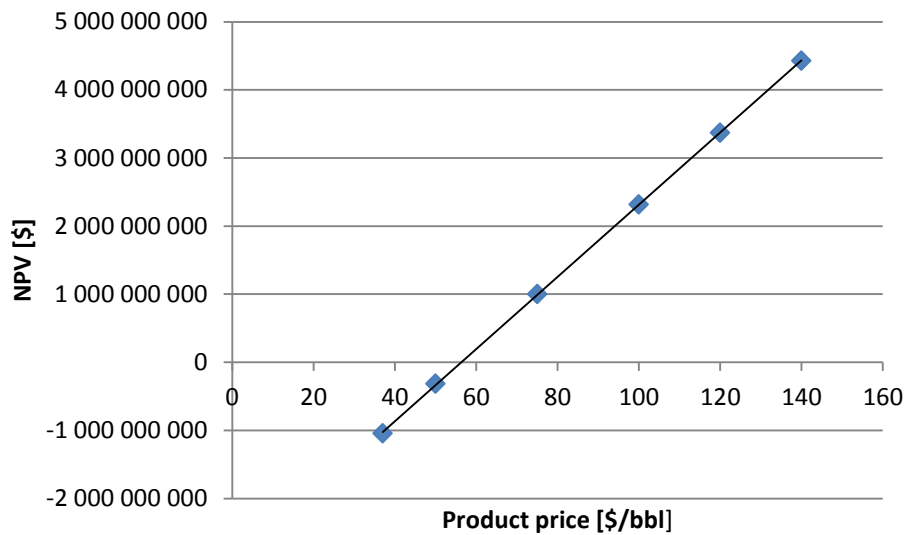


Figure 18 - NPV vs. product prices

As seen from Figure 18, the average product price has to be at least 57 \$/bbl to make this project profitable at the given natural gas price.

6.3 Tax rate

The tax rate is an uncertain factor and was set to 30% throughout the project. A change in tax rate affects the profitability as seen in Figure 19.

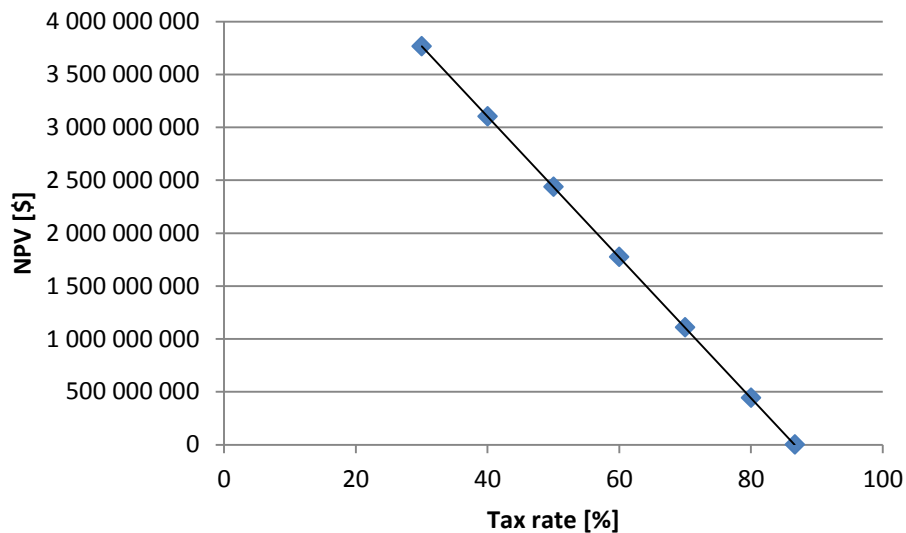


Figure 19 - NPV vs. Tax rate

As seen from Figure 19, the project will reach break even if the tax rate is 86.7%.

6.4 Historic progress

The graph below shows how the profitability of the project would have been in different years, assumed that the prices would have been stable for the whole lifetime. Figure 20 shows the ten last years. The data, which this graph is made of, are collected from figures in Appendix B.

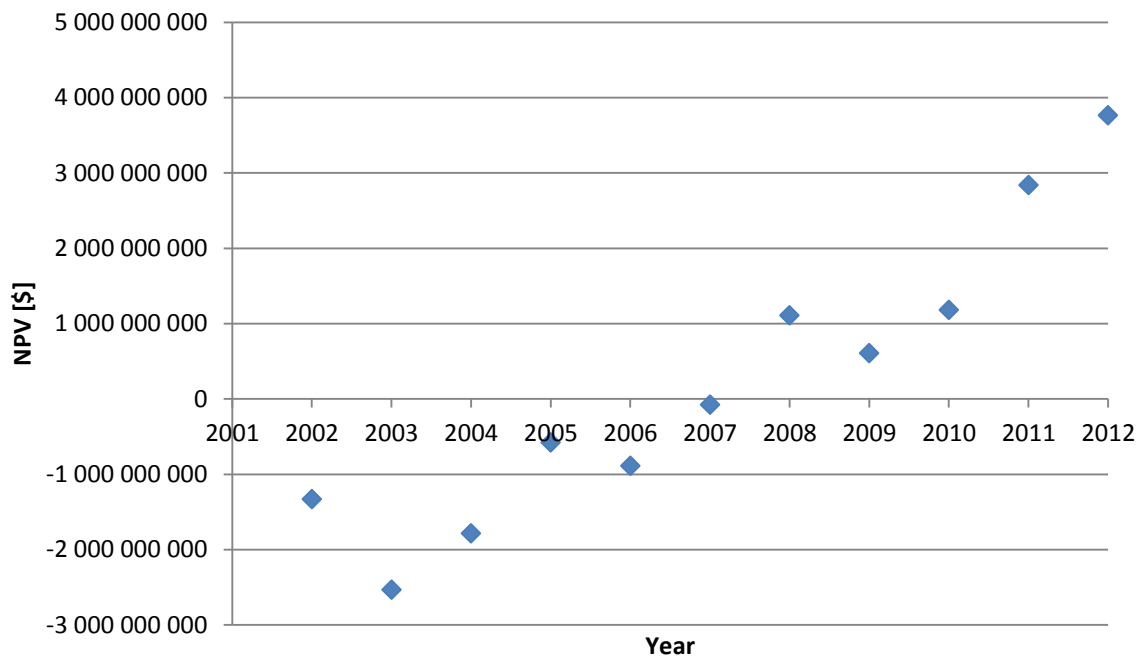


Figure 20 - Historic NPV progress

As seen from Figure 20 the project would not have been profitable before 2008, with the assumptions made. The trend here is that a GTL plant seems to be more profitable in the future, but there are large uncertainties.

7. Discussion

7.1 Assumptions

In the model there were assumed that all reactions happened in vapor phase. Key numbers from HYSYS showed that this was a good assumption because 97 vol% of the inlet gas was in vapor phase and along the reactor where cracking and isomerization took place the vapor fraction increased due to lower boiling point on cracked and isomerized products.

The energy was not conserved in the simulation. This was due to the lumping of components from MATLAB to HYSYS. When sending back values to HYSYS all iso-compounds higher than 10 had to be lumped in to one new lump called i-C₁₀₊ due to the lack of components in the HYSYS databank. Doing this lead to loss of information regarding heat flow and thus the energy balance was not conserved. If the energy balance was corrected for this loss of information (stream 18 and stream 19 was included), the error would be 0.11% of the inlet stream. This error was due to the recycle loops in HYSYS which all contained a small error, and the simplifications made in the model. This meant that the assumption of all reaction in vapor phase and the neglected terms in the temperature equation (see Appendix C), was reasonable and the magnitude of the results was not affected significantly.

The lumping of components gives less accuracy than a more complete model, but an “all component model” will still be inaccurate due to different properties of all isomers with same carbon number. The lumped kinetics model is a simple model which gives a pointer at the final product distribution, and needs less computational time and power which have been limited in this project.

7.2 Optimization

With a high H₂/wax ratio, the profitability went down. This can be explained by equations 3.9-3.11.

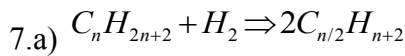
$$r_{iso} = \frac{k_{iso} \left(p_{n-c} - \frac{p_{iso-c}}{K_{eq}} \right) - k_{cr} p_{iso-c}}{ADSORB} \quad (3.9)$$

$$r_{cr} = \frac{k_{cr} p_{iso-c}}{ADSORB} \quad (3.10)$$

$$ADSORB = p_{H_2} \left[1 + \sum_i K_{L_{n-c,i}} p_{n-c,i} + K_{L_{iso-c,i}} p_{iso-c,i} \right] \quad (3.11)$$

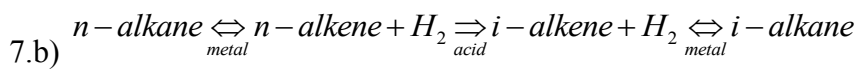
A high H₂/wax ratio leads to high hydrogen partial pressure which slows the reaction rates. As seen from equations above a large hydrogen amount will increase the partial pressure of hydrogen, which again will increase the ADSORB term and lead to slower reaction rates. Since the reaction rates are given per m³ this signifies that a larger reactor volume is needed to get the wanted outlet distribution. High H₂/wax ratios imply that more hydrogen is needed which leads to higher investment cost since the hydrogen plant must be larger and higher production costs due to the operation of the hydrogen plant.

If the H₂/wax ratio is too low, the hydrogen limits the reaction, and the reactor outlet still has a large fraction of heavy hydrocarbons which have not been cracked. This can be seen by equation 7.a below, which is a cracking reaction. This reaction is irreversible, and the reaction will stop if all hydrogen is consumed.

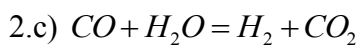


Heavy hydrocarbons are not as valuable as the middle distillate as seen from Table 17, and thus the profitability will be lower.

The optimal H₂/wax ratio found in chapter 4.3.3 is not necessarily optimal because the ratio between iso and normal paraffins are not taken into account. Isomerization reactions neither produce nor consume hydrogen, but the hydrogen added may shift the equilibrium as seen in equation 7.b (46).



When the LPG stream was recycled back to the pre-reformer instead of purged, a slightly higher internal rate of return was achieved. The reason why it was only slightly higher was that the LPG stream contained a lot of CO₂ (48 wt%) which reversed the WGS reaction in the pre-reformer and ATR.



That led to a H_2/CO ratio different from the wanted value of two. To counteract this reversion, more steam had to be injected to shift the equilibrium towards right again. This meant that steam which could have been sold had to be used in the process instead. More steam and recycling increased the size of equipment in addition to an extra compressor which had to be installed.

Since both isomerization and cracking reactions are exothermic, high temperature had positive effect on the reaction rates. As seen from Figure 9 there was a temperature interval which was desirable. If the temperature got too low, the reaction rates were slow, and a huge reactor volume was needed to achieve the wanted outlet distribution. If the temperature got too high, installation and operation of the fired heater would be expensive, and it would be harder to control the outlet distribution due to the fast reaction rates. This could lead to more cracking than wanted, so the outlet products would mainly be LPG and naphtha which were not that valuable.

The reaction rates are inversely proportional to the partial pressure of hydrogen as seen from equations 3.9-3.11 above. An increase in total pressure would increase the partial pressure of hydrogen, and this would lead to slower isomerization reactions as seen from equation 3.9 and 7.b. The dehydrogenation step would be shifted towards n-alkanes. Lowering the pressure would benefit both isomerization and cracking of all lumps (20). Lower pressures would affect the selectivity of the cuts, but this was controlled by temperature instead.

Optimizing manually with holding all other variables constant while changing one can lead to “wrong” optimized value. With so many design variables there’s a possibility that local peaks were found and not global peak. If the global peak was to be found, a plot of all design variables and the net present value had to be made. Alternatively an optimization routine in another program could have been used.

7.3 Economics

The fixed capital investment cost was 790 million dollars for a 24 000 bbl/day capacity plant. This was reasonable compared to the ORYX plant owned by Sasol and Qatar Petroleum. That plant had an investment cost of 1 billion dollars in 2006 for a 34 000 bbl/day capacity (18), which would be 1.17 billion dollars in 2011 price when taking the CEPCI into account. Both plants used slurry reactors and cobalt catalysts, so they were comparable.

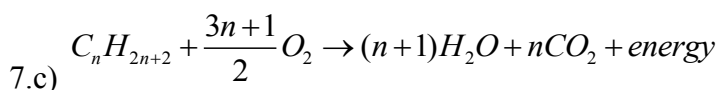
There were large uncertainties in the cost of the ASU and H₂ plant. The ASU was scaled up from an existing plant and the cost of the H₂ plant was scaled from a cost found in a report. These two accounted for most of the capital cost and changes in them would affect the capital investment cost most.

The production costs were highly influenced by the natural gas price. The natural gas was assumed bought in this project. To get the natural gas as cheap as possible, there is an advantage if the plant was in a remote area. In remote areas the gas could be cheaper due to the lack of other options. Making pipelines and transporting it far away would be more expensive, than selling for a lower price to another immediate company.

The ASU had potential to separate oxygen, nitrogen and argon (47). Nitrogen and argon could be sold, and that was not taken into account, thus the income could have been higher.

In the economic analysis there was assumed the owners of the plant had enough funds to start up, without borrowing money. This was a weak assumption, and the profitability would be lower if the project had to be financed by loan, cause then there would be rates on the loan.

Another factor which was not considered in the economics was emission costs. The purge gas was assumed to be fuel for the fired heaters. The hydrocarbons would combust to CO₂ after equation 7.c. This is an exothermic reaction so energy would be released in form of heat (48).



According to Bellona (49) the cost for CO₂ emissions is below 20 euros/ton CO₂. If this was added in the economic result, the production cost would increase with 8.5 million dollars each year and give an IRR of 0.63 percentage points lower (see Appendix F). This meant that neglecting the cost of CO₂ emission was not a huge mistake.

The internal rate of return was 52%, which indicated that this was a very beneficial project. The return on investment was 53%, and denoted that the gain was 53% of the investment cost each year. These values presumed that the natural gas price, electricity price, product prices etc. would be stable for a period of twenty years, and that no equipment had to be replaced. The last assumption is plausible if the design and material selection is made thoroughly. The first assumption is improbable as natural gas price and product prices change each day. For the ten

last years (see Appendix B) there have been vigorous changes in these, and it is likely that significant changes will appear for the coming 20 years.

7.4 Sensitivity analysis

From the sensitivity analysis it could be seen that the plant was robust against an increase in natural gas price. This was due to the high product prices at the moment. Figure 28, Figure 29 and Figure 30 in Appendix B show that natural gas price and product prices are unstable, and there's possible that the project will be unprofitable for some of the years during the expected lifetime.

The tax rate was uncertain and was set to 30% from past report (18). Only income taxes were considered. A study of a GTL plant in Alaska had more detailed values. There it was assumed 2% property tax, 9.40% State Corporate Income Tax and 35% Federal Corporate Income Tax (50). In that case the profitability would have been significantly lower. Income taxes would be 44.40% in addition to property tax. As seen from Figure 19, the NPV would be around 2.5-3 billion dollars. This plant was assumed to be at the Gulf Coast, but the fact is that most GTL plants are located in Qatar due to the large gas reserves. If the plant was in Qatar, a flat tax rate of 10% is the reality. This rate was set to encourage foreign investors. Before 2010 it was 35% (51). With a tax rate of 10% the NPV would have been much higher, if all other factors were equal.

From Figure 20 it could be seen that startup year for the project was of significance. A lot of assumptions were made to draw that figure. The prices for natural gas and products were assumed stable for the whole lifetime, which is a wrong assumption. The investment costs were not corrected by CEPCI, all prices were 2011 prices. The point of this figure was to illustrate that huge deviations can occur from year to year, and it is impossible to foresee the prices in the future from past data. This means that even though the project seems highly profitable at the moment, it can be unprofitable over a period of 20 years due to an unstable market.

7.5 Material selection

The steam/carbon ratio into the ATR was fairly low (0.56), thus it is important to study further on the ATR, to avoid side reaction, which can make soot formation appear after equation 7.d. Especially the burner design should be studied further (2).

$$7.d) \quad C_n H_m = nC + \frac{m}{2} H_2$$

Soot formation could also be a problem in the pre-reformer, where carbon whisker tends to grow with a nickel crystal at the top (2). Soot formation leads to catalyst deactivation and is favored at high temperatures and low steam/carbon ratio.

The temperature in the ATR and out of the ATR is so high that other material than stainless steel should be considered to avoid metal dusting. Metal dusting is a severe form of corrosion that occurs when a material is in an environment with high carbon activity. The corrosion can break up bulk metal to metal powder which interferes with the process. A mechanism to avoid metal dusting is to protect the metal with a chromium layer (52).

7.6 Environmental discussion

Since this is a gas plant, there will be some emission of gases, mainly CO₂. The content of sulfur and aromatics is small, and compared to other options, fuels from oil or coal, a GTL plant is eco-friendly.

Installing a CO₂ removal unit was considered, but according to Bellona (49), this will not be economically profitable at the current time. For a carbon capture and storage unit to be profitable the emission allowances must exceed 35 EUR/ton CO₂. At the moment it is below 20. The technology behind these units are still in development, but Bellona claims that such units can be profitable after 2025, presumed that the emission allowances are above 35 EUR/ton CO₂. Earlier reports have shown that a post combustion CO₂ removal unit in a GTL plant, which removed 60-70% of the CO₂, was slightly profitable, but there a cost of 50\$/ton CO₂ removed was used (18).

8. Conclusion

- The most beneficial inlet temperature to the hydrotreater was found to be 335 °C, and an inlet pressure of 25 bars.
- A H₂/wax ratio of 0.14 seemed to be an optimal value, and this implied that the hydrotreater must be at least 33 m³ for the wanted outlet distribution.
- For the stream named 'LPG', a case study was done. The study showed that it was most profitable to recycle that stream back to the pre reformer. This led to higher carbon efficiency and higher net present value of the project.
- The project was highly profitable at today's prices, with a net present value of 3.8 billion dollars, using a discount rate of 9% and a horizon of 20 years.
- The internal rate of return was 52%, and the return on investment (calculated as an average over the horizon) was 53%.
- The sensitivity analysis showed that the project was beneficial with natural gas price up to 13 \$/MMbtu, as long as the product prices did not decrease.
- The lumping of components between MATLAB and HYSYS led to loss of information regarding heat flow, which caused the energy balance to not conserve.

List of symbols

Symbol	Definition	Unit
A	Area	m ²
a	Cost constant	
b	Cost constant	
C	Cost	US\$
C _p	Specific heat capacity	kJ/(kgmole*K) , kJ/(kg*K)
D	Diameter of reactor	m
d _p	Diameter of particle	m
E	Activation energy	kJ/kgmole
F	Molar flow	kgmole/h
f	Friction factor	
f (subscript)	Installation factors	
H	Enthalpy	kJ/mole
h	Height	m
i	Discount rate	
I	CEPCI value	
k	Reaction rate constant	kmole/(kg*h) , kmole/(Pa ^{1.25} *m ³ *s)
K	Henry's law constants	Pa ⁻¹
K _{eq}	Equilibrium constant	
L	Length	m
M	Molar mass	kg/kgmole
m*	Mass flow	kg/h , ton/day
n	Cost exponent	
N	Number of something (operators, equipment etc.)	
p	Partial pressure	Pa , bar
P	Total pressure	bar
Q	Heat flow	kW
R	Universal gas constant	J/(mole*K)
r	Reaction rate	kgmole/(m ³ *s) , kgmole/(kg _{cat} *h)
Re	Reynolds number	

S	Size parameter	m^2 , kg , kW etc.
T	Temperature	K , °C
t	Thickness	m
U	Overall heat transfer coefficient	$\text{W}/(\text{m}^2 \cdot ^\circ\text{C})$
V	Volume	m^3
V*	Volume flow	m^3/h , bbl/day
v^s	Superficial velocity	m/s
xc	Currency conversion	NOK/US\$, £/\$
y	Mole fractions	mole/mole
z	Length	m
α	Chain growth probability	
γ	Lump fraction	
ε	Void fraction	$\text{m}^3_{\text{catalyst}}/\text{m}^3_{\text{reactor}}$
μ	Viscosity	cP
ρ	Density	kg/m^3
σ	Stress	ksi
σ^*	Surface tension	mN/m
τ	Residence time	h
Ψ	Generalized quantity	bar , K , etc.
ω	Mass fractions	kg/kg

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Appendix A – Cost calculation/ equipment sizing

This appendix will show calculation of the equipment cost. The general formula for calculating the prices of the equipment is given in equations 5.1-5.3. The C values given in tables below are 2011 values for stainless steel, and are the same values which can be found in Table 14 in the main report.

A.1 Heat exchangers

There were three heat exchangers shown on the flowsheet. In fact there were other heat exchangers as well, because the first one, E-101, was four heat exchangers in series as shown in Figure 22. All heat exchangers were modeled as U-tube shell and tube exchangers, where the size parameter was the area in m². The U-values (overall heat transfer coefficients) were found in Table 12.1 in Sinnott (41). The UA value was found from HYSYS and then the area was calculated by Equation A.1.

$$A = \frac{UA}{U} \quad (\text{A.1})$$

To find the optimal design for E-101, a pinch analysis was performed as seen in Figure 21. See flowsheet (Figure 1) to see where stream 5 and HP steam are.

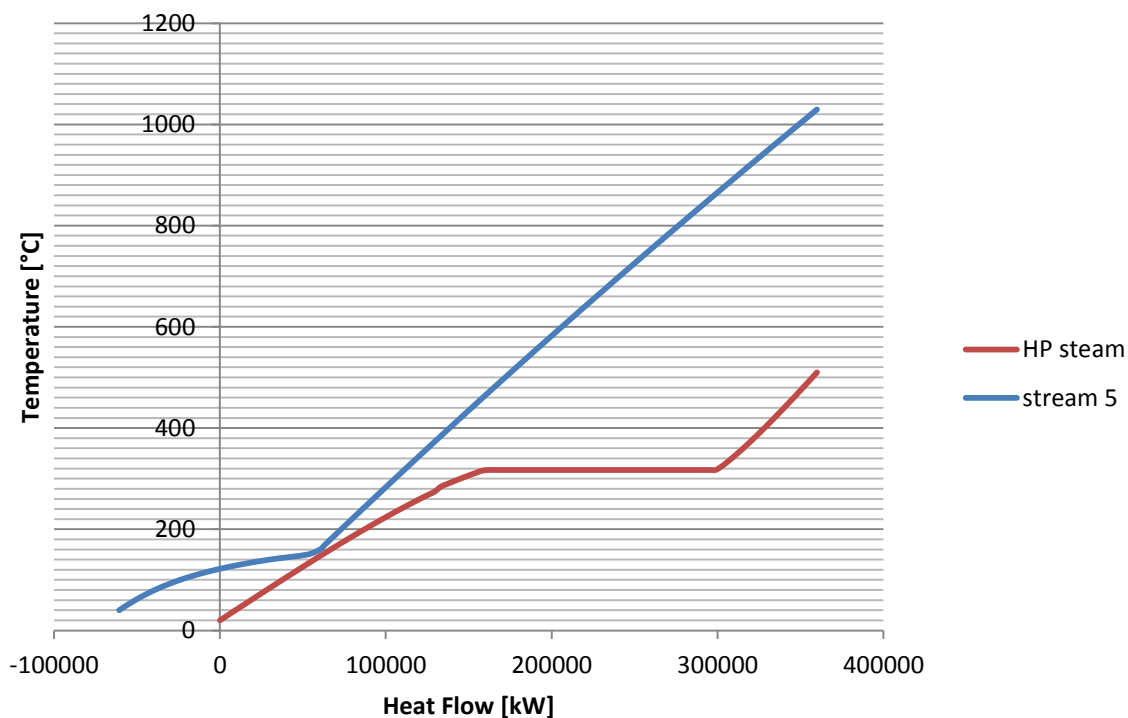


Figure 21 - Pinch analysis

The minimum temperature difference, ΔT_{\min} , was set to 10 °C. As seen from the figure, external cooling water was needed in order to cool down the rest of the fluid (the part on negative heat flow side). The set-up for this exchanger network is given in Figure 22.

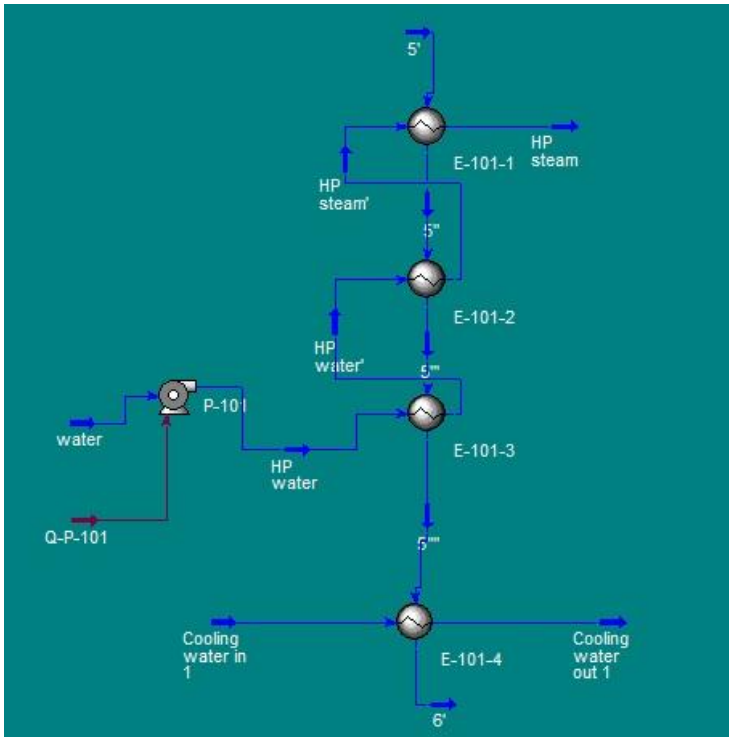


Figure 22 - Heat exchanger network

The area was calculated from equation A.1, and all four exchangers were added.

The second heat exchanger, E-102, used HP steam to heat up the fluid as seen in Figure 23. The temperature in to the FT reactor was set to 210 °C. A lower inlet temperature was considered, because then LP steam could be used for heating. This was not done, because large amounts of oxygenates could be formed. At higher temperatures the methane selectivity greatly increases (53).

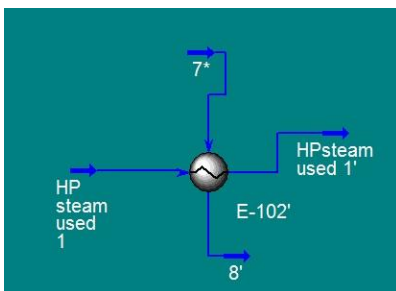


Figure 23 - E-102

The third exchanger, E-103, used cooling water to cool the fluid mixture down to wanted temperature as seen in Figure 24. The fluid should reach 30 °C at the outlet of the exchanger.

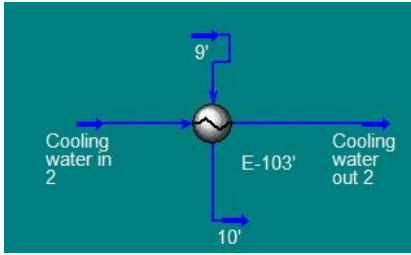


Figure 24 - E-103

A summary of the cost of all heat exchangers are given in Table 18.

Table 18 - Heat exchangers

Tag name	U [W/(m ² *°C)]	A [m ²]	a	b	n	C ₂₀₁₁ [million US\$]
E-101	750	6 349	24000	46	1.2	9.6
E-102	1000	589	24000	46	1.2	0.7
E-103	750	3 778	24000	46	1.2	5.2

A.2 Cooling tubes

Inside the Fischer-Tropsch reactor there were several cooling tubes to cool the mixture and make low pressure steam. To find the cost of the cooling tubes, the duty and temperatures from HYSYS were used, and the area was found from equation A.2.

$$Q = UA\Delta T_{lm} \quad (\text{A.2})$$

Then the total length of tubes was found from equation A.3

$$A = \pi LD \quad (\text{A.3})$$

The diameter of the tubes was approximately 5 centimeters (9). When the length of the tubes was found, a correlation in literature (54) said that the price was approximately 2 \$/feet of tube (1991 price). The total price of the tubes became 1.6 million US\$.

A.3 Pressure vessels

All reactors, separators and steam drums were modeled as pressure vessels in stainless steel. For the separators and steam drums a residence time of five minutes was assumed (41). Further a height/diameter ratio of 3 was assumed for all pressure vessels (42) if nothing else is specified in the text.

A.3.1 Separators and steam drums

The volume of separators and steam drums were calculated from equation A.4. The steam drums are not shown on flowsheet, but they were needed when steam was produced, and is located along with E-101 and FT reactor

$$V = \frac{V^*}{\tau} \quad (\text{A.4})$$

Where V is the volume [m³], V* is the volume flow [m³/h] and τ is the residence time [h].

Assuming the vessels were cylindrical, the diameter can be found from equation A.5 where the height was substituted with diameter (h=3D).

$$D = \left(\frac{4V}{3\pi} \right)^{\frac{1}{3}} \quad (\text{A.5})$$

To find the cost of the vessels the shell mass was needed, and in order to find the shell mass the thicknesses had to be found. The thicknesses of the vessels were found using equation 13.40 in Sinnott (41), given as equation A.6 below.

$$t = \frac{P_i D}{2\sigma - P_i} \quad (\text{A.6})$$

Where t is the wall thickness, P_i is the design pressure which is 10% larger than the actual pressure and σ is the maximum allowable stress. The maximum allowable stress was found from a temperature dependency in Table 13.2 in Sinnott (41). When the thicknesses were found, the shell mass could be found from equation A.7.

$$m = t\rho(2\pi rh + 4\pi r^2) = t\rho\pi(Dh + D^2) \quad (\text{A.7})$$

The first term represents the mass of the sidewalls and the second part represents the mass of the ends. There were assumed hemispherical ends.

Table 19 - Separators and Steam drums

	Water Separator	3-phase Separator	Steam drum 1	Steam drum 2
Tag name	V-101	V-102	-	-
Modeled as	Vertical pressure vessel	Horizontal pressure vessel	Vertical pressure vessel	Vertical pressure vessel
V [m ³]	90	172	33	43
D [m]	3.4	4.2	2.4	2.6
P _i [bar]	30.4	28.2	121	11
T [°C]	30	30	510	190
σ [ksi]	21	21	10.8	14
t [m]	0.036	0.041	0.216	0.015
m [kg]	40 847	72 420	125 795	10 454
a	10 000	8 800	10 000	10 000
b	29	27	29	29
n	0.85	0.85	0.85	0.85
C ₂₀₁₁ [million US\$]	1.4	2.1	3.6	0.5

A.3.2 Reactors

There were four reactors in the plant. The two first (pre-reformer and ATR) were modeled as equilibrium reactors, so there was not possible to optimize the volume of them in HYSYS, because there would not be any changes in the streams when volume was changed. Therefore the size of them was set. The pre-reformer was assumed to have a diameter of 4 meters and was 6 meters high, while the ATR was assumed to be 8 meters in diameter and 6 meters high (55).

The Fischer-Tropsch reactor was optimized in an earlier project, and the optimal volume was found to be 2700 m³ (13). The volume of the hydrotreater was found to be 33 m³ as seen in Chapter 4.2.4. The same equations were used to find the shell mass for the reactors as for the separators and steam drums. The different parameters are summarized in Table 20.

Table 20 - Reactors

	Pre-reformer	ATR	FT reactor	Hydrotreater
Tag name	R-101	R-102	R-103	R-104
Modeled as	Vertical pressure vessel	Vertical pressure vessel	Vertical pressure vessel	Vertical pressure vessel
V [m ³]	75	302	2700	33
D [m]	4.0	8.0	10.5	2.4
P _i [bar]	32.6	31.5	29.3	29.7
T [°C]	465	1030	210	354
σ [ksi]	11.7	11.5	14	16.2
t [m]	0.083	0.163	0.162	0.033
m [kg]	83 296	458 373	1 421 458	19 023
a	10 000	10 000	10 000	10 000
b	29	29	29	29
n	0.85	0.85	0.85	0.85
C ₂₀₁₁ [million US\$]	2.5	10.6	27.7	0.8

A.4 Distillation column

The distillation column was modeled as a vertical pressure vessel made of stainless steel. The column used valve trays inside, i.e. the Koch Flexitray (56). A picture of the Koch Flexitray is given in Figure 25 below. The benefits of these trays are a uniform vapor distribution and they are cost effective (57).

**Figure 25 - Koch Flexitray**

The column was modeled as three shortcut columns in HYSYS (see Figure 26)

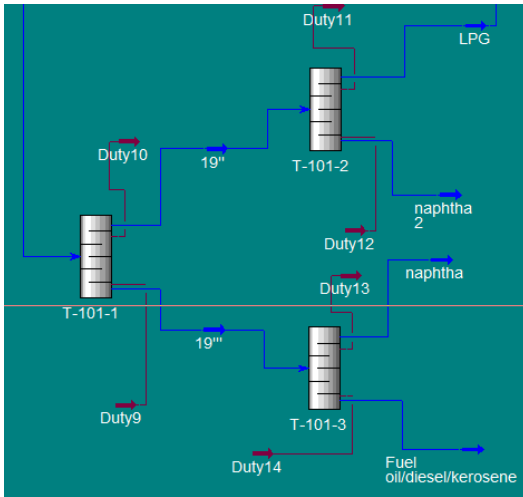


Figure 26 - Distillation column

The height of the column was estimated from the actual number of trays in HYSYS, which were 85. The spacing between stages was set to 0.5 meters (approximately 20 inches) (58). In addition 15 % extra disengaging space was needed in top and bottom of the column (58). This gave a total height of 49 meters.

The diameter was estimated from equations and Figure 11.5-3 in Geankoplis (59) (given as Figure 31 in Appendix B). The values needed from HYSYS are given in Table 21.

Table 21 - Parameters needed to estimate column diameter

Parameter	Value	Unit	Meaning
m_v^*	$1.30 \cdot 10^4$	kg/h	Mass flow vapor
m_L^*	$1.16 \cdot 10^5$	kg/h	Mass flow liquid
ρ_v	13.09	kg/m ³	Density vapor
ρ_L	296.7	kg/m ³	Density liquid
σ^*	0.7259	mN/m	Liquid surface tension

The first step was to determine the K_v value. This was done in Figure 11.5-3 in Geankoplis (59), and it was found to be 0.067 feet/s. After that the allowable vapor velocity was calculated from equation A.8.

$$v_{\max} = K_v \left(\frac{\sigma^*}{20} \right)^{0.2} \sqrt{\frac{\rho_L - \rho_V}{\rho_V}} \quad (\text{A.8})$$

Using this equation the v_{\max} was 0.16 feet/s. Then the design velocity could be calculated.

$$v_{\text{design}} = v_{\max} (0.91 \cdot 0.95 \cdot 0.80) \quad (\text{A.9})$$

To account for the downspout area, the velocity was multiplied by 0.91. 0.95 for foaming and 0.80 for 80% of flooding. The design velocity was 0.11 feet/s = 0.034 m/s. Then the cross sectional area could be found using equation A.10.

$$A = \frac{m_v^*}{3600 \frac{\text{s}}{\text{h}}} \cdot \frac{1}{\rho_V} \cdot \frac{1}{v_{\text{design}}} \quad (\text{A.10})$$

And at last the diameter could be found using equation A.11

$$d_c = \sqrt{\frac{4A}{\pi}} \quad (\text{A.11})$$

The column diameter was estimated to 3.22 meters.

The thickness and shell mass was found using equations A.6 and A.7. The thickness was 0.033 meters and the shell mass was 131 571 kg.

The cost of the column was then estimated from equations 5.1-5.3, and the values are given in Table 22. The size parameter for the column was the shell mass in kg and for the trays it was the column diameter in meters.

Table 22 - Distillation column

Tag name	a	b	n	S	C ₂₀₁₁ [million US\$]
T-101	10000	29	0.85	131 571 kg	
Valve Trays	180	340	1.9	3.22 m	
Total cost					5.3

A.4.1 Reboiler and Condenser

As seen from Figure 26, the reboiler and condenser had to be calculated from six different energy streams. The reboiler and condenser were both calculated from three heat exchangers each, where the areas were added together. The network can be seen in Figure 27.

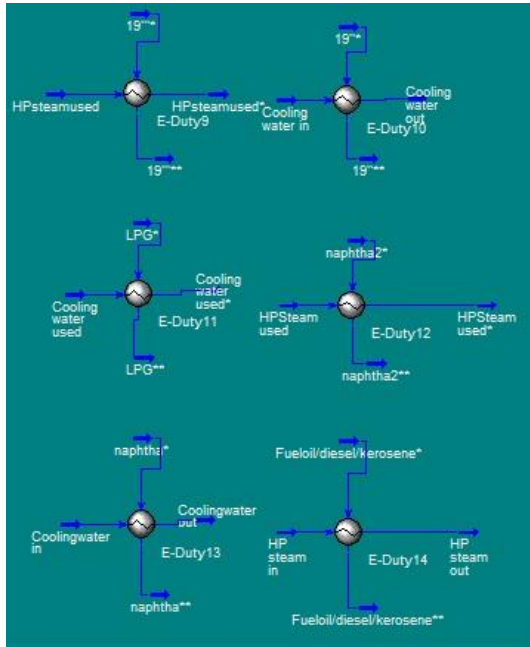


Figure 27 - Reboiler and Condenser network

The areas were found using equation A.1. A summary is given in Table 23. The reboiler was modeled as a U-tube kettle reboiler and the condenser as a U-tube shell and tube.

Table 23 - Reboiler and Condenser

Equipment	A [m ²]	U [W/(m ² *°C)]	a	b	n	C ₂₀₁₁ [million US\$]
Condenser	57	500	24000	46	1.2	0.2
Reboiler	145	750	25000	340	0.9	0.3

A.5 Compressors

For compressors the size parameter for estimation was driver power in kW. The costs of all compressors are summarized in Table 24. All compressors were centrifugal.

Table 24 - Compressors

Tag name	a	b	n	S [kW]	C ₂₀₁₁ [million \$]
C-101	490000	16800	0.6	1 945	11.6
C-102	490000	16800	0.6	171	4.8
C-103	490000	16800	0.6	311	5.7

A.6 Fired heaters

There were two fired heaters in the plant. The first one, H-101, was modeled as a box furnace, while the other one, H-102, was modeled as a cylindrical furnace. This was because the validity of the two types was different. The size parameter was the duty in MW. A summary of the cost are given in Table 25.

Table 25 - Fired heaters

Tag name	a	b	n	Q [MW]	C ₂₀₁₁ [million US\$]
H-101	37 000	95 000	0.8	112	23.5
H-102	68 500	93 000	0.8	34	9.1

A.7 Pumps

The pumps are not shown on flowsheet, but they were needed in order to make high and low pressure steam. The first pump can be seen in Figure 22, while the other pump was used to pump up the water used inside the cooling tubes in the FT reactor. Both pumps were modeled as single-stage centrifugal pumps, and the size parameter was the flow given in L/s. Table 26 summarizes the costs of the two pumps.

Table 26 - Pumps

Tag name	a	b	n	S [L/s]	C ₂₀₁₁ [million US\$]
P-101	6900	206	0.9	109	0.1
P-102	6900	206	0.9	142	0.1

A.8 ASU

The cost of the air separation unit was 125 000 000 NOK (2001 price) for a 325 ton O₂/day, with a scaling factor of 0.7. The energy demand was 0.8 kWh/kg O₂ (14). In this plant there was 4030 ton/day used. The price for this ASU in 2011 can be calculated from equation A.12.

$$C_{ASU,2011} [\$] = C_{ASU,2001} [NOK] \cdot \left(\frac{I_{2011}}{I_{2001}} \right) \cdot \left(\frac{m_{actual}^*}{m_{ref}^*} \right)^n \cdot \left(\frac{1}{xc} \frac{US\$}{NOK} \right) = \quad (A.12)$$

$$125\,000\,000 \cdot \left(\frac{585.7}{394.3} \right) \cdot \left(\frac{4029.6}{325} \right)^{0.7} \cdot \left(\frac{1}{5.82638} \right) = 185\,662\,698 US\$$$

Where the I represents the Chemical Engineering's Plant Cost Index (CEPCI) and xc represents the currency conversion between NOK and US\$.

A.9 H2 plant

The cost of the hydrogen plant was 130 998 000 \$ (2000 price) for a 417.8 ton/day plant. In addition there was a power consumption of 6 MW and a cost of 5.54 \$/MMbtu of hydrogen produced (44). In this plant there was 180 ton/day hydrogen needed. The investment cost could then be calculated according to equation A.13.

$$C_{H_2 plant, 2011} [\$] = C_{H_2 plant, 2000} \cdot \left(\frac{I_{2011}}{I_{2000}} \right) \cdot \left(\frac{m_{actual}^*}{m_{ref}^*} \right)^n = \quad (A.13)$$

$$130998000 \cdot \left(\frac{585.7}{394.1} \right) \cdot \left(\frac{180}{417.8} \right)^1 = 83875964 US\$$$

The scaling factor here was not known, so it was assumed to be 1.

A.10 Catalyst

The catalyst cost was the sum catalysts in all four reactors. In the pre-reformer and ATR there were nickel catalyst used, which had a price of 100 NOK/liter (55). In the FT reactor there was cobalt catalyst which had a price of 30 \$/lb for finished catalyst (60). In the hydrotreater there was amorphous silica-alumina consisted of platinum and γ -alumina binder (12) which had a price of 12 \$/lb (40). In the first three reactors the void fraction was set to 0.1 according to the maximum allowed concentration of catalyst (18). In the hydrotreater the void fraction was 0.8 (20). The void fraction could be much higher there due to the advantages of a trickle bed reactor. A summary of the catalyst cost is given in Table 27.

Table 27 - Catalyst cost

Used in	Type of catalyst	Catalyst cost	Void fraction	C ₂₀₁₁ [million US\$]
Pre-reformer	Nickel based	100 NOK/liter	0.1	0.1
ATR	Nickel based	100 NOK/liter	0.1	0.5
FT reactor	Cobalt based	30 \$/lb	0.1	35.7
hydrotreater	Silica-alumina	12 \$/lb	0.8	0.8

Appendix B – Figures and charts

This appendix shows the graphs and charts which were used to get the results in the report. To convert 1 barrel equals approximately 42 gallons.

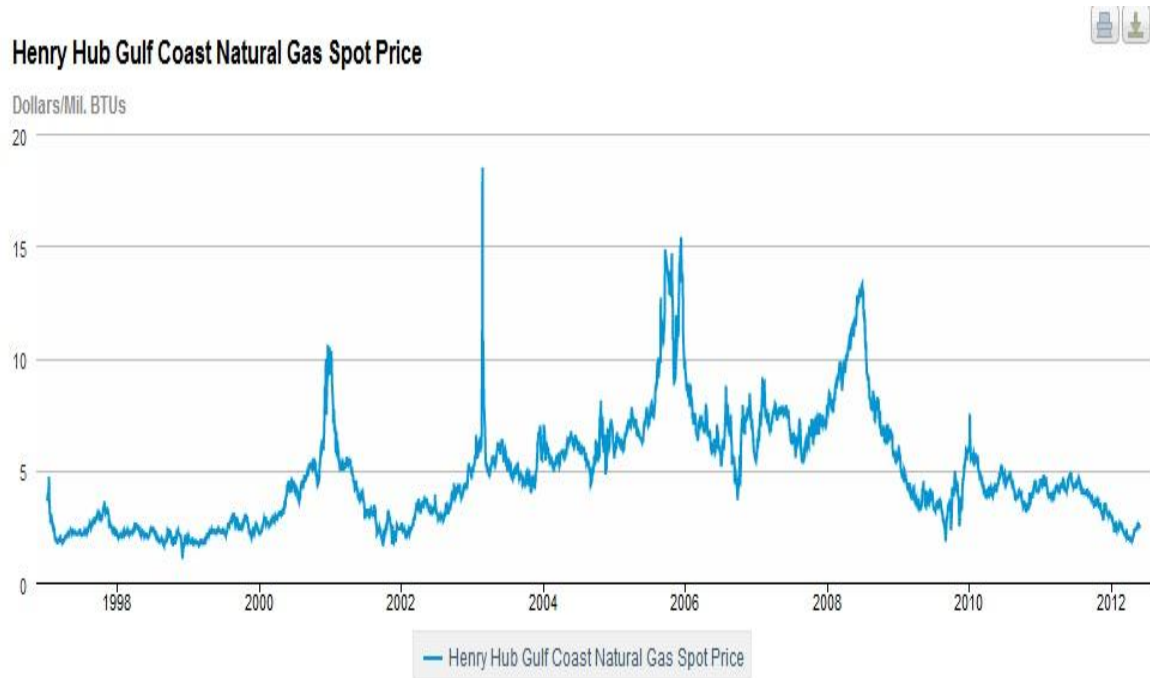


Figure 28 - Natural gas price (43)

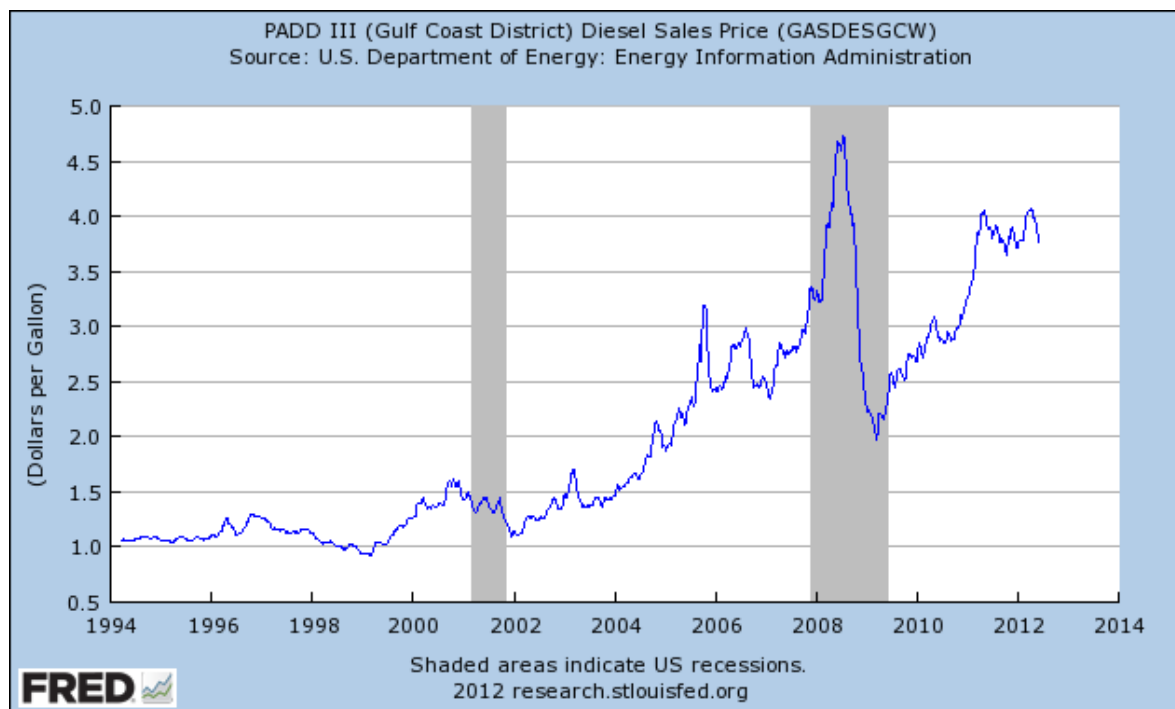
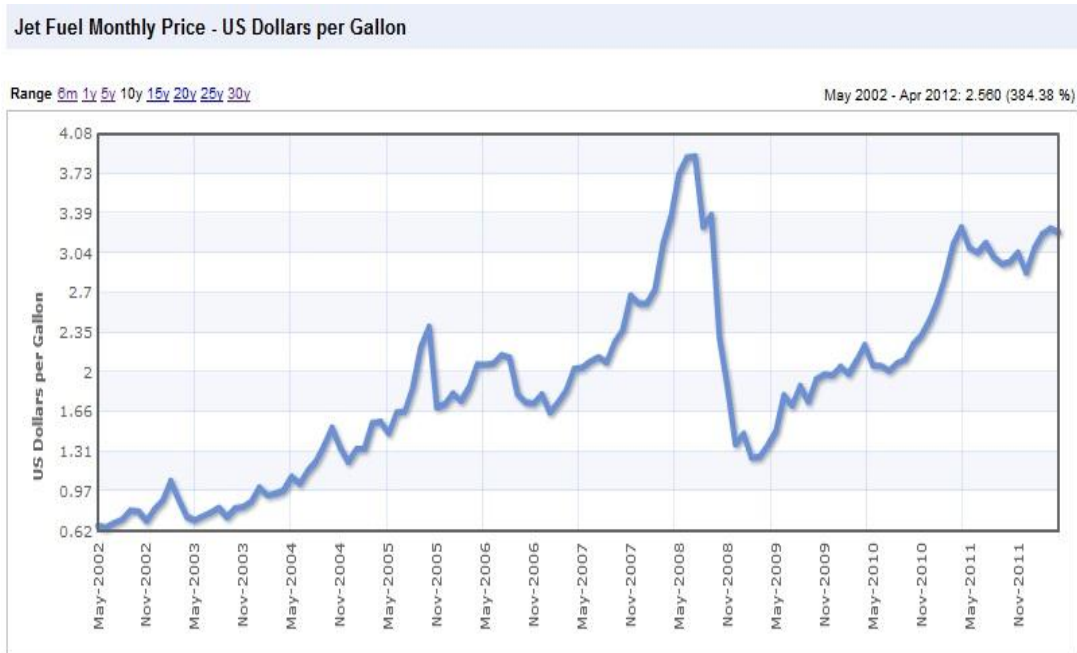


Figure 29 - Diesel price (61)



Description: U.S. Gulf Coast Kerosene-Type Jet Fuel Spot Price FOB

Figure 30 - Jet fuel/kerosene price (62)

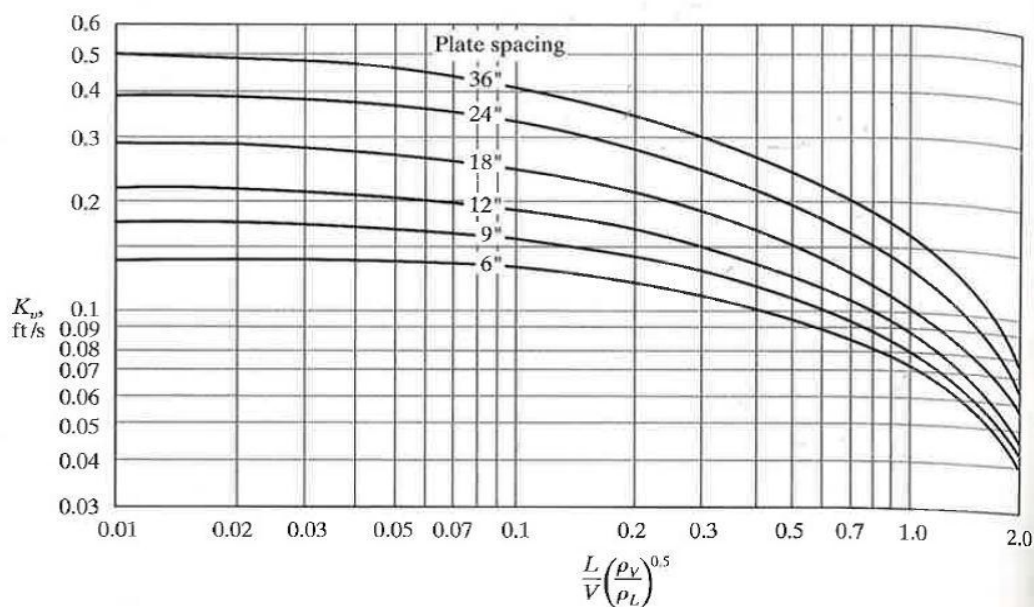


FIGURE 11.5-3. Estimation of K_v value for allowable vapor velocity. (From Fair, J. R., Petro/Chem. Eng., 33(10), 45 (1961). With permission.)

Figure 31 - Estimation of K_v value (59)

Appendix C – Derivation of equations

This appendix shows a complete view of the derivation of the equations. The derivation is taken from Jakobsen (36).

Mass balance:

General equation:

$$\frac{\partial}{\partial t}(\rho\omega_s) + \nabla \cdot (\rho \underline{v} \omega_s) = -\nabla \cdot \underline{j}_s + R_s \quad (3.5)$$

The first term on the left hand side denotes the mass gained by time (if dynamic system). The second term on the left hand side denotes the rate of mass gained by convective mass transport. The first term on the right hand side is the rate of mass by conductive mass transport. The second term on the right hand side is mass gained by chemical reaction.

Convective transport is completely dominant over the diffusive term, because the fluid moves like a plug, and thus the diffusive term can be neglected (36). No effects of inter/intra-particle diffusion because of powdered catalyst (12).

Because of axisymmetric, convective gradients will only occur in z-direction

Then the equation reduces to

$$\frac{\partial}{\partial t}(\rho\omega_s) + \frac{\partial}{\partial z}(\rho v^s \omega_s) = R_s \quad (C.1)$$

Assuming steady state conditions, the transient term disappears

$$\frac{\partial}{\partial z}(\rho v^s \omega_s) = R_s \quad (C.2)$$

Multiplying by the cross sectional area, A, on both sides

$$\frac{\partial}{\partial z}(A\rho v^s \omega_s) = AR_s \quad (C.3)$$

Using the relations

$$Av^s = \dot{V} \quad (C.4)$$

And

$$\dot{V}\rho = \dot{m} \quad (C.5)$$

The equation reduces to

$$\frac{\partial}{\partial z}(\dot{m}\omega_s) = AR_s \quad (C.6)$$

Dividing by the area again on both sides, the equation becomes

$$\frac{\partial \omega_s}{\partial V} = \frac{R_s}{\dot{m}} \quad (C.7)$$

Using the relation between reaction rates on molar and mass basis,

$$R_s = M_s \sum_j \nu_{ij} r_j \quad (C.8)$$

The final equation can be written as

$$\frac{d\omega_s}{dV} = \frac{M_s}{\dot{m}} \sum_j \nu_{ij} r_j \quad (3.7)$$

Temperature equation

General equation

$$\begin{aligned} \rho C_{p, mass} \left(\frac{\partial T}{\partial t} + \underline{v} \cdot \nabla T \right) = -\nabla \cdot \underline{q} - \frac{T}{\rho} \left(\frac{\partial \rho}{\partial T} \right)_{p, \omega} \frac{Dp}{DT} \\ -\underline{\sigma} : \nabla \underline{v} + \sum_{s=1}^n \frac{\bar{h}_s}{M_s} \nabla \cdot \underline{j}_s + \sum_{r=1}^Q \frac{R_r}{M_{A_{ref}}} (-\Delta H_{rx, r}) \end{aligned} \quad (3.6)$$

Left hand side:

The first term denotes the rate of gain of heat by time. The second term denotes the rate of heat gained by convective heat transport.

Right hand side:

The first term denotes the energy input by conductive heat transport (radiation). The second term denotes the work done by surrounding pressure due to fluid motion. The third term is irreversible rate of internal energy by viscous dissipation. The fourth term denotes inter-diffusion energy flux. The fifth term denotes heat by chemical reaction

Heat conduction is much smaller than heat convection, and can thus be neglected. Steady state simulation is applied, so the transient term can be neglected. The reactor is axisymmetric, so only flow in z-direction is considered. Pressure and viscous forces are neglected. No external cooling/heating and no effects of inter-diffusion due to powdered catalyst (12).

Using this assumptions, and the relation

$$MC_{p, mass} = C_{p, molar} \quad (C.9)$$

The equation reduces to

$$\rho \frac{\tilde{C}_{p, molar}}{\tilde{M}} v \frac{\partial T}{\partial z} = \sum_{r=1}^Q r_r (-\Delta H_{rx, r}) \quad (C.10)$$

Multiplying by A on both sides

$$A \rho \frac{\tilde{C}_{p, molar}}{\tilde{M}} v \frac{\partial T}{\partial z} = A \sum_{r=1}^Q r_r (-\Delta H_{rx, r}) \quad (C.11)$$

Using the relations

$$Av = \dot{V} \quad (C.4)$$

And

$$\dot{V} \rho = \dot{m} \quad (C.5)$$

The final equation becomes

$$\frac{dT}{dV} = \frac{\tilde{M}}{\dot{m} \tilde{C}_{p, molar}} \sum_{r=1}^Q r_r (-\Delta H_{rx, r}) \quad (3.8)$$

Where \tilde{M} and $\tilde{C}_{p, molar}$ are mean values.

Appendix D – MATLAB

To calculate the values in the ASF distribution, formulas given in Hillestad (25) and MATLAB were used. The formulas needed are given below.

$$p_i = (1 - \alpha)^2 \alpha^{i-1} \quad (\text{D.1})$$

$$U' = 3 - \alpha \quad (\text{D.2})$$

$$\sum_{i=1}^{\infty} i p_i = 1 \quad (\text{D.3})$$

Equation D.2 and D.3 are used to calculate p_i and U' , and the last equation is to make sure that the sum adds up to 1 according to the weight ASF distribution (25).

The MATLAB script is given below.

```
%-----ASF.m-----  
%-----Ole Kristian Nordvåg-----  
%-----22.05.2012-----  
  
clear all  
clc  
format long  
  
%Rx: CO + UH2 --> p1C1 + p2C2 + ... + p20C20 +sum(pnuCnu) + H2O  
%ASF distribution  
alfa=0.90;  
N=21;  
  
%average carbon number of lump  
Xnu=N+(alfa/(1-alfa))  
U=3-alfa  
%calculating pi values  
  
for i=1:N-1  
    p(i)=(1-alfa)^2*(alfa^(i-1));  
end  
  
for i=N:999  
    pnu(i)=(1-alfa)^2*(alfa^(i-1));  
end  
  
disp (p)
```

```

pn=sum(pnu)

%checking if the sum adds up to 1
for i=1:999
    p(i)=(1-alfa)^2*(alfa^(i-1));
    y(i)=sum(i*p(i));
end
Y=sum(y(1:i))

```

The rest of the MATLAB scripts were used to solve the equations in the hydrotreater

```

%-----constant.m-----
%-----Ole Kristian Nordvåg-----
%-----22.05.2012-----

global Vend

R=8.314;                %Universal gas constant [kJ/(kmol*K)]

%Modelling and Optimization of Fischer-Tropsch products hydrocracking,
%Fernandes, Teles Fuel processing Technology 88 2007
rhocat=950;            %kg/m3reactor    rhocat*epsilon

%Modelling of FT products hydrocracking
%Pellegrini, Calemma ....
%Model 1
my5=(1/2);
my5star=(1/3);
my6=(9/16);

%Kliso [Pa-1]
Kliso59=5.46e0;
Kliso1014=5.48e1;
Kliso1522=9.46e2;
Kliso22=9.53e7;

%Kln [Pa-1]
Kln14=5.46e-2;
Kln59=5.47e0;
Kln1014=5.48e1;
Kln1522=9.05e2;
Kln22=7.19e7;

```

```

%Keq []
Keq59=7.19e2;
Keq1014=8.36e2;
Keq1522=3.76e3;
Keq22=5.73e3;

%k0iso [kmol/(h*m3)]
k0iso59=1.14e23;
k0iso1014=2.60e24;
k0iso1522=9.47e27;
k0iso22=2.80e29;

%k0cr [kmol/(h*m3)]
k0cr59=4.48e22;
k0cr1014=9.50e24;
k0cr1522=7.05e26;
k0cr22=7.90e27;

%Eiso [kJ/kmol]
Eiso59=1.94e5;
Eiso1014=1.94e5;
Eiso1522=1.94e5;
Eiso22=2.06e5;

%Ecr [kJ/kmol]
Ecr59=1.30e5;
Ecr1014=1.66e5;
Ecr1522=1.82e5;
Ecr22=1.87e5;

%the all component hydrocracking model
%Model 2
% my5=(1/2);
% my5star=(1/3);
% my6=(9/16);

%Kliso [Pa-1]
% Kliso59=5.46e0;
% Kliso1014=5.48e1;
% Kliso1522=9.46e2;
% Kliso22=9.53e7;
%
% Kln [Pa-1]

```

```

% Kln14=5.46e-2;
% Kln59=5.47e0;
% Kln1014=5.48e1;
% Kln1522=9.05e2;
% Kln22=7.19e7;
%
% %Keq []
% Keq59=3.59e3;
% Keq1014=3.78e3;
% Keq1522=3.86e3;
% Keq22=5.93e3;
%
% %k0iso [kmol/(h*m3)]
% k0iso59=1.14e23;
% k0iso1014=7.60e24;
% k0iso1522=9.47e27;
% k0iso22=2.80e29;
%
% %k0cr [kmol/(h*m3)]
% k0cr59=4.48e22;
% k0cr1014=4.50e24;
% k0cr1522=3.05e26;
% k0cr22=2.99e27;
%
% %Eiso [kJ/kmol]
% Eiso59=1.61e5;
% Eiso1014=1.68e5;
% Eiso1522=1.92e5;
% Eiso22=2.01e5;
%
% %Ecr [kJ/kmol]
% Ecr59=1.34e5;
% Ecr1014=1.65e5;
% Ecr1522=1.85e5;
% Ecr22=1.93e5;
%-----
Vend=33;
dp=3e-3;
dt=2*((Vend/6/pi)^(1/3));
epsilon=0.8;
A=pi*dt*dt/4;
h=Vend/A;

%Volume of reactor [m3]
%diameter of catalyst particle [m]
%diameter of reactor tube [m]
%void fraction
%Area of tube [m2]
%Height of reactor

%-----Reactorinlet.m-----

```

```

%-----Getting values from HYSYS----
%-----Ole Kristian Nordvåg-----
%-----22.05.2012-----

format short

h=actxserver('HYSYS.Application');           %Create an interface
hyCase=h.Activedocument;                   %between MATLAB and HYSYS
Sol=hyCase.Solver;
f=hyCase.Flowsheet;
g=f.Materialstreams;
Sol.CanSolve=1;

%Atom matrix
%  1  2  3    4    5    6    7    8    9
%[H2 CO CO2  H2O  nC1-4  nC5-9  nC10-14  nC15-20  nC21+

%10    11    12    13
%iC5-9  iC10-14  iC15-20  iC21+]

%Mass fractions at inlet
win=g.Item('18').componentMassFractionValue;
win=[win(26) win(28:29) win(25) win(1:3) win(5) win(7:23) win(30)
(0.1152/0.5452)*win(31) (0.22/0.5452)*win(31) (0.21/0.5452)*win(31)];
Win=sum(win);

%Total flows at inlet
Min=g.Item('18').MassFlowValue;              %Total mass
flow [kg/s]
Fin=g.Item('18').MolarFlowValue;             %Total mole
flow in [kmole/s]
Vin=g.Item('Flash out vapor').ActualVolumeFlowValue; %Actual volume
flow [m3/s]

%Molecular weight of the mixture
Mmix=g.Item('18').MolecularweightValue;

%Temperature in
Tin=273.15+g.Item('18').TemperatureValue;    %Temperature
at inlet [K]

%Pressure in
pin=1000*g.Item('18').PressureValue;         %Pressure
inlet [Pa]

```

```

%Mass density
    rhogasfeed=g.Item('Flash out vapor').MassDensityValue; %Mass density
at inlet [kg/m3]

%Gas viscosity
    mygas=(1/1000)*g.Item('Flash out vapor').ViscosityValue; %Dynamic
viscosity [Pa*s]
%-----enthalpiesandCp.m-----
%Standard enthalpies and specific heat capacity values
%-----Ole Kristian Nordvåg-----
%-----22.05.2012-----

%Enthalpies [kJ/kgmole]
DH0C14=(1/4)*(-74900-84738-103890-126190); %HYSYS
DH0C59=(1/5)*(-146490-167290-187890-208590-229190); %HYSYS
DH0C1014=(1/5)*(-249790-270490-291090-311690-332290); %HYSYS
DH0C1520=(1/6)*(-352990-373590-394190-414780-435390-456080); %HYSYS
DH0C30=-664200; %HYSYS
DH0iC59=-192390; %HYSYS, i-C7,
3methylhexane
DH0iC1014=-295200; % Hopfe, D. Data
Compilation of FIZ CHEMIE, Germany , p. 28 (1990) %iC12, 5Mundecane
DH0iC1520=-419700; %same ref as above
%iC18, 2Mheptadecane
DH0iC30=-864700; %Zhang, F.M.; Xu,
G.D.; Qu, S.S., Studies on thermochemistry of porphyrins V...
%The standard energies of combustion and standard enthalpies of formation of
bromoporphyrin compounds, Acta Chimica Sinica, 1990, 48, 38-41. [all data]
%iC30, squalane, liquid heat of formation
DH0H2=0; %HYSYS
DH0CO=-110590; %HYSYS
DH0CO2=-393790; %HYSYS
DH0H2O=-241814; %HYSYS

DH0=[DH0H2 DH0CO DH0CO2 DH0H2O DH0C14 DH0C59 DH0C1014 DH0C1520 DH0C30 DH0iC59
DH0iC1014 DH0iC1520 DH0iC30];

%Heat capacities (at 25 C) [kJ/(kgmole*K)]
CpC14=(1/4)*(36+53+74+97); %SI
CpC59=(1/5)*(120+143+166+189+212); %SI
CpC1014=280; %SI, dodecane
CpC1520=515.8; %HYSYS, octadecane
CpC30=960.4; %HYSYS

```



```

CpIC59=210.9; %HYSYS, iC7, 3Mhexane
CpIC1014=372; %Hopfe+++as above, iC12,
5Mundecane
CpIC1520=536; %Hopfe+++,iC18,
2Mheptadecane
CpIC30=886.36; %iC30, squalane Trejo,
L.M.; Costas, M.; Patterson, D., Excess heat capacity of organic mixtures,
Internat...
% DATA Series, Selected
Data Mixt., 1991, Ser. [all data]
CpH2=29; %SI
CpCO=29; %SI
CpCO2=37; %SI
CpH2O=34; %SI

Cp=[CpH2 CpCO CpCO2 CpH2O CpC14 CpC59 CpC1014 CpC1520 CpC30 CpIC59 CpIC1014 CpIC1520
CpIC30];

%-----MMass.m-----
%Molecular weights of the different components [kg/kmol]
%-----Ole Kristian Nordvåg-----
%-----22.05.2012-----

Reactorinlet

MMH2=2.016;
MMCO=28.0109;
MMCO2=44.0097;
MMH2O=18.0151;
MMC1=16.0429;
MMC2=30.0699;
MMC3=44.0970;
MMC4=58.1240;
MMC5=72.1510;
MMC6=86.1779;
MMC7=100.205;
MMC8=114.232;
MMC9=128.259;
MMC10=142.285;
MMC11=156.313;
MMC12=170.339;
MMC13=184.367;
MMC14=198.380;
MMC15=212.410;
MMC16=226.429;

```

```

MMC17=240.457;
MMC18=254.479;
MMC19=268.510;
MMC20=282.540;
MMC30=422.799;

MMnC14=1/((1/(sum(win(5:8))))*(win(5)/MMC1+win(6)/MMC2+win(7)/MMC3+win(8)/MMC4));
MMnC59=1/((1/(sum(win(9:13))))*(win(9)/MMC5+win(10)/MMC6+win(11)/MMC7+win(12)/MMC8+win(13)/MMC9));
MMnC1014=1/((1/(sum(win(14:18))))*(win(14)/MMC10+win(15)/MMC11+win(16)/MMC12+win(17)/MMC13+win(18)/MMC14));
MMnC1520=1/((1/(sum(win(19:24))))*(win(19)/MMC15+win(20)/MMC16+win(21)/MMC17+win(22)/MMC18+win(23)/MMC19+win(24)/MMC20));
MMnC30=MMC30;
MMiC59=MMnC59;
MMiC1014=MMnC1014;
MMiC1520=MMnC1520;
MMiC30=MMnC30;

MMi=[MMH2 MMCO MMCO2 MMH2O MMnC14 MMnC59 MMnC1014 MMnC1520 MMnC30 MMiC59 MMiC1014 MMiC1520 MMiC30];

%-----loser.m-----
%-----Solving the equations-----
%-----Ole Kristian Nordvåg-----
%-----22.05.2012-----

function dbdV = loser(V,b)

global Vend

MMass
constant
Reactorinlet
enthalpiesandCp

T0=298.15;
w=b(1:13);
T=b(14);
ptot=b(15);
Mmix=1/(sum(w./MMi'));
W=sum(w)
yi=w.*Mmix./MMi';
Y=sum(yi);

```

```

massin2=Min.*3600;      %mass in [kg/h]

pri=yi.*ptot;           %partial pressure of each component

Adsorb=pri(1)*(1+Kln22*pri(9)+Kliso22*pri(13)+Kln1522*pri(8)+Kliso1522*pri(12)...
    +Kln1014*pri(7)+Kliso1014*pri(11)+Kln59*pri(6)+Kliso59*pri(10)+Kln14*pri(5));

%reaction rates [kmol/(kgcat*h)]
if (pri(1)>0)
    r1=k0iso22*exp(-Eiso22/R/T)*(pri(9)-(pri(13)/Keq22))/Adsorb;
    r2=k0iso1522*exp(-Eiso1522/R/T)*(pri(8)-(pri(12)/Keq1522))/Adsorb;
    r3=k0iso1014*exp(-Eiso1014/R/T)*(pri(7)-(pri(11)/Keq1014))/Adsorb;
    r4=k0iso59*exp(-Eiso59/R/T)*(pri(6)-(pri(10)/Keq59))/Adsorb;
    r5=k0cr22*exp(-Ecr22/R/T)*pri(13)/Adsorb;
    r6=k0cr1522*exp(-Ecr1522/R/T)*pri(12)/Adsorb;
    r7=k0cr1014*exp(-Ecr1014/R/T)*pri(11)/Adsorb;
    r8=k0cr59*exp(-Ecr59/R/T)*pri(10)/Adsorb;
else                                     %if/else is only used to make the
simulation                               %converge when all hydrogen is consumed
    r1=0;
    r2=0;
    r3=0;
    r4=0;
    r5=0;
    r6=0;
    r7=0;
    r8=0;
end

%MASS BALANCES
%-----
rn22=-r1;
riso22=r1+(1-my5-my5star)*r5-(my5+my5star)*r5;
rn1522=-r2;
riso1522=r2+2*my5*r5-my6*r6-(1-my6)*r6;
rn1014=-r3;
riso1014=r3+2*(1-my6)*r6+2*my5star*r5-r7;
rn59=-r4;
riso59=r4+2*r7+2*my6*r6-r8;
rn14=2*r8;
rH2=-(my5+my5star)*r5-r6-r7-r8;

% %dwi/dV [1/m3]
dwdVn1=MMi(5)*rhocat/massin2*rn14;          %nC1-4
dwdVn2=MMi(6)*rhocat/massin2*rn59;          %nC5-9

```

```

dwdVn3=MMi(7)*rhocat/massin2*rn1014;           %nC10-14
dwdVn4=MMi(8)*rhocat/massin2*rn1522;           %nC15-20
dwdVn5=MMi(9)*rhocat/massin2*rn22;             %nC21+
dwdVi1=MMi(10)*rhocat/massin2*riso59;          %iC5-9
dwdVi2=MMi(11)*rhocat/massin2*riso1014;        %iC10-14
dwdVi3=MMi(12)*rhocat/massin2*riso1522;        %iC15-20
dwdVi4=MMi(13)*rhocat/massin2*riso22;          %iC21+
dwdVH2=-(dwdVn1+dwdVn2+dwdVn3+dwdVn4+dwdVn5+dwdVi1+dwdVi2+dwdVi3+dwdVi4);
dwdVCO=0;
dwdVCO2=0;
dwdVH2O=0;

%ENERGY BALANCE
%-----
Cpm=sum(Cp*w);
DHf=DH0+Cp*(T-T0);

%Isomerisation reactions
DHrx1=(DHf(13)-DHf(9))*r1;
DHrx2=(DHf(12)-DHf(8))*r2;
DHrx3=(DHf(11)-DHf(7))*r3;
DHrx4=(DHf(10)-DHf(6))*r4;

%Cracking reactions
DHrx5=(2*my5*DHf(12)-my5*DHf(13)-DHf(1))*r5;
DHrx6=(2*(1-my6)*DHf(11)-(1-my6)*DHf(12)-DHf(1))*r6;
DHrx7=(2*DHf(10)-DHf(11)-DHf(1))*r7;
DHrx8=(2*DHf(5)-DHf(10)-DHf(1))*r8;
DHrx9=(2*my5star*DHf(11)-my5star*DHf(13)-DHf(1))*r5;
DHrx10=(2*my6*DHf(10)-my6*DHf(12)-DHf(1))*r6;

DHrx=[DHrx1 DHrx2 DHrx3 DHrx4 DHrx5 DHrx6 DHrx7 DHrx8 DHrx9 DHrx10];

dTdV=rhocat*Mmix/massin2/Cpm*-(sum(DHrx));

%%Pressure equation (Ergun's equation)
%-----
rhogas=ptot*Mmix/R/T/1000;                      %gas density [kg/m3]
vs=Vin/A;                                         %Superficial gas velocity
[m/s]
Re=vs*dp*rhogas/mygas;                          %Reynolds number []
fric=(1-epsilon)/(epsilon^3)*(1.75+(150*(1-epsilon)/Re)); %friction factor

dPdV=-fric*rhogas*vs*vs/dp/A;                   %Pressure loss [Pa/m3]

```

```

dbdV=[dwdVH2 dwdVCO dwdVCO2 dwdVH2O dwdVn1 dwdVn2 dwdVn3 dwdVn4 ...
      dwdVn5 dwdVi1 dwdVi2 dwdVi3 dwdVi4 dTdV dpdV]';

%-----main.m-----
%-----odesolver and plotting-----
%-----Ole Kristian Nordvåg-----
%-----22.05.2012-----

global Vend

constant      %Calling other files
MMass
Reactorinlet

step=1;
Vspan=[0:step:Vend];
b0=[win(1:4) sum(win(5:8)) sum(win(9:13)) sum(win(14:18)) sum(win(19:24)) win(25)
win(26) win(27) win(28) win(29) Tin pin]';    %boundary conditions
nc=length(b0);

[V,b]=ode45(@loser,Vspan,b0)

for i=1:(Vend/step+1)
    MMix(i)=1/(sum(b(i,1:13)./MMi));
    y(i,:)=b(i,1:13).*MMix(i)./MMi;
    wnc(i,:)=b(i,5:9);
    wic(i,:)=b(i,10:13);
    ync(i,:)=y(i,5:9);
    yic(i,:)=y(i,10:13);
end

%Plotting
%-----
figure(1)
plot(V,b(:,5:13))
legend('C1-4','C5-9','C10-14','C15-20','C21+', 'iC5-9','iC10-14','iC15-20','iC21+');
set(legend,'Location','North')
title('mass fractions of hydrocarbons')
xlabel('Volume [m3]')
ylabel('mass fractions')

figure(2)
plot(V,b(:,1:13))

```

```

legend('H2','CO','CO2','H2O','C1-4','C5-9','C10-14','C15-20','C21+', 'ic5-9','ic10-14', 'ic15-20','ic21+');
set(legend,'Location','Northeast')
title('mass fractions of all components')
xlabel('Volume [m3]')
ylabel('mass fractions')

figure(3)
plot(V,b(:,14)-273.15)
legend('T');
set(legend,'Location','North')
title('Temperature plot')
xlabel('Volume [m3]')
ylabel('Temperature [C]')

figure(4)
plot(V,b(:,15)/100000)
legend('ptot');
set(legend,'Location','North')
title('Pressure plot')
xlabel('Volume [m3]')
ylabel('Total pressure [bar]')

LPG=b(end,5)
naphta=b(end,6)+b(end,10)
kerosene=b(end,7)+b(end,11)
diesel=b(end,8)+b(end,12)
fueloil=b(end,9)+b(end,13)

wout=[0 0 b(end,5) 0 0 0 0 0 b(end,6) 0 0 0 0 b(end,7) 0 0 0 0 0 b(end,8) 0
0 b(end,9) 0 b(end,4) b(end,1) 0 b(end,2) b(end,3) b(end,10)
sum(b(end,11)+b(end,12)+b(end,13))]

pause

%Sending values back to HYSYS
%-----
g.Item('C1-4').TemperatureValue=b(end,14)-273.15;
g.Item('C1-4').PressureValue=b(end,15)/1000;
g.Item('C1-4').MassflowValue=Min*wout(3);
g.Item('C5-9').TemperatureValue=b(end,14)-273.15;
g.Item('C5-9').PressureValue=b(end,15)/1000;
g.Item('C5-9').MassflowValue=Min*wout(9);
g.Item('C10-14').TemperatureValue=b(end,14)-273.15;
g.Item('C10-14').PressureValue=b(end,15)/1000;

```

```

g.Item('C10-14').MassflowValue=Min*wout(14);
g.Item('C15-20').TemperatureValue=b(end,14)-273.15;
g.Item('C15-20').PressureValue=b(end,15)/1000;
g.Item('C15-20').MassflowValue=Min*wout(20);
g.Item('C21+').TemperatureValue=b(end,14)-273.15;
g.Item('C21+').PressureValue=b(end,15)/1000;
g.Item('C21+').MassflowValue=Min*wout(23);
g.Item('iC5-9').TemperatureValue=b(end,14)-273.15;
g.Item('iC5-9').PressureValue=b(end,15)/1000;
g.Item('iC5-9').MassflowValue=Min*wout(30);
g.Item('iC10+').TemperatureValue=b(end,14)-273.15;
g.Item('iC10+').PressureValue=b(end,15)/1000;
g.Item('iC10+').MassflowValue=Min*wout(31);
g.Item('H2').TemperatureValue=b(end,14)-273.15;
g.Item('H2').PressureValue=b(end,15)/1000;
g.Item('H2').MassflowValue=Min*wout(26);
g.Item('H2O').TemperatureValue=b(end,14)-273.15;
g.Item('H2O').PressureValue=b(end,15)/1000;
g.Item('H2O').MassflowValue=Min*wout(25);
g.Item('CO').TemperatureValue=b(end,14)-273.15;
g.Item('CO').PressureValue=b(end,15)/1000;
g.Item('CO').MassflowValue=Min*wout(28);
g.Item('CO2').TemperatureValue=b(end,14)-273.15;
g.Item('CO2').PressureValue=b(end,15)/1000;
g.Item('CO2').MassflowValue=Min*wout(29);

```


Appendix E – HYSYS

This appendix shows the flowsheet and workbook from the HYSYS simulation with LPG recycle. To get a better view and understanding the .hsc files for both cases are given in Appendix F.

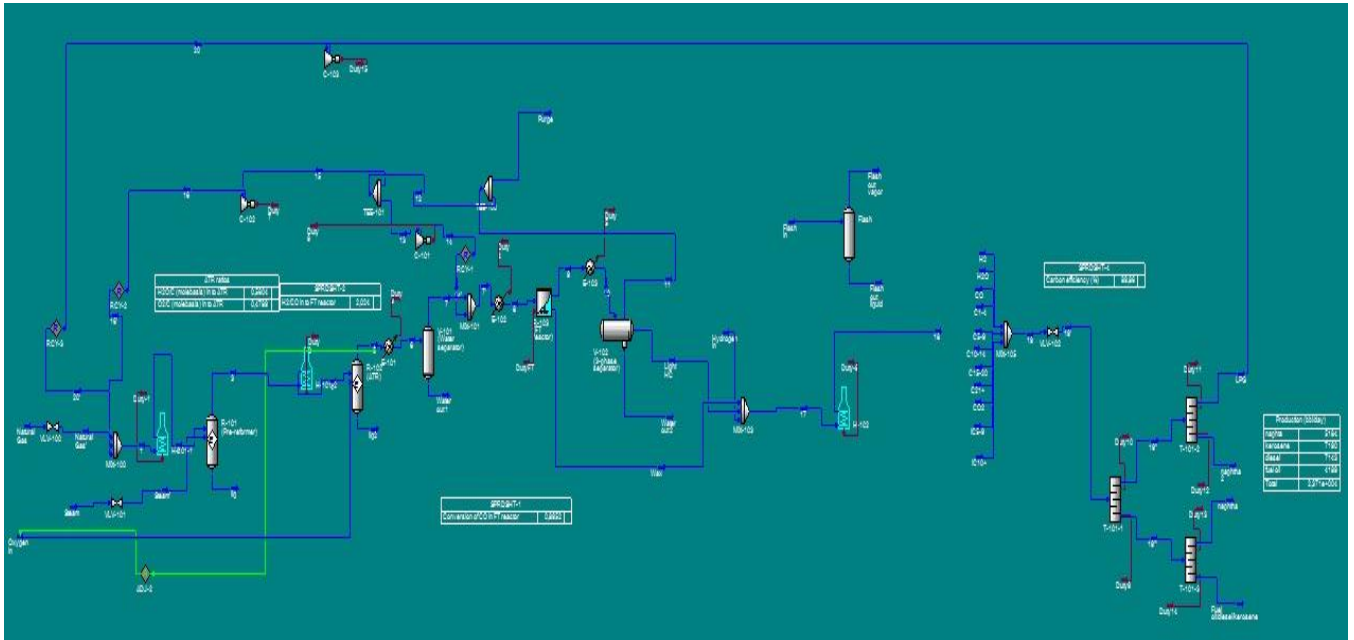


Figure 32 - HYSYS flowsheet

aspen		NORWEGIAN UNIV OF Burlington, MA USA		Case Name: FERDIG2 RECYCLE.HSC		
				Unit Set: Oleekte		
				Date/Time: Tue Jun 12 09:00:31 2012		
Workbook: Case (Main)						
Material Streams				Fluid Pkg:		All
Name	Natural Gas	Natural Gas'	1	2	3	
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000	
Temperature (C)	50.00 *	41.40	44.65	455.0 *	457.9	
Pressure (kPa)	5000 *	3000 *	3000	2965	2965	
Molar Flow (kgmole/h)	8218 *	8218	1.025e+004	1.025e+004	1.811e+004	
Mass Flow (kg/h)	1.434e+005	1.434e+005	2.037e+005	2.037e+005	3.299e+005	
Liquid Volume Flow (m3/h)	456.2	456.2	558.5	558.5	726.6	
Heat Flow (kW)	-1.746e+005	-1.746e+005	-2.985e+005	-2.380e+005	-6.791e+005	
Name	liq	Steam	4	5	liq2	
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	0.0000	
Temperature (C)	457.9	510.0 *	650.0 *	1030	1030	
Pressure (kPa)	2965	1.100e+004 *	2865	2865	2865	
Molar Flow (kgmole/h)	0.0000	7000 *	1.811e+004	3.629e+004	0.0000	
Mass Flow (kg/h)	0.0000	1.261e+005	3.299e+005	4.978e+005	0.0000	
Liquid Volume Flow (m3/h)	0.0000	126.4	726.6	1080	0.0000	
Heat Flow (kW)	0.0000	-4.412e+005	-6.275e+005	-6.199e+005	0.0000	
Name	Oxygen in	6	7	Water out 1	8	
Vapour Fraction	1.0000	0.8051	1.0000	0.0000	1.0000	
Temperature (C)	200.0 *	30.00 *	30.00	30.00	210.0 *	
Pressure (kPa)	2865 *	2765	2765	2765	2665	
Molar Flow (kgmole/h)	5247 *	3.629e+004	2.922e+004	7072	6.023e+004	
Mass Flow (kg/h)	1.679e+005	4.978e+005	3.702e+005	1.275e+005	1.508e+006	
Liquid Volume Flow (m3/h)	147.6	1080	952.0	127.8	2634	
Heat Flow (kW)	7518	-1.045e+006	-4.835e+005	-5.616e+005	-2.889e+006	
Name	9	Wax	10	11	Light HC	
Vapour Fraction	1.0000	0.0000	0.7819	1.0000	0.0000	
Temperature (C)	210.0 *	210.0	30.00 *	30.00	30.00	
Pressure (kPa)	2665	2665	2565	2565	2565	
Molar Flow (kgmole/h)	4.280e+004	175.1	4.280e+004	3.347e+004	608.1	
Mass Flow (kg/h)	1.452e+006	5.634e+004	1.452e+006	1.228e+006	6.471e+004	
Liquid Volume Flow (m3/h)	2066	70.17	2066	1816	89.94	
Heat Flow (kW)	-3.258e+006	-2.407e+004	-3.467e+006	-2.723e+006	-4.965e+004	
Name	Water out 2	Purge	7'	12	16	
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	1.0000	
Temperature (C)	30.00	30.00	30.45	30.00	43.75	
Pressure (kPa)	2565	2565	2765	2565	3000 *	
Molar Flow (kgmole/h)	8727	1171	6.023e+004	3.230e+004	1292	
Mass Flow (kg/h)	1.587e+005	4.299e+004	1.508e+006	1.185e+006	4.742e+004	
Liquid Volume Flow (m3/h)	159.6	63.56	2634	1753	70.10	
Heat Flow (kW)	-6.946e+005	-9.529e+004	-3.004e+006	-2.627e+006	-1.049e+005	
Name	16'	15	13	14	14'	
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000	
Temperature (C)	43.75 *	30.00	30.00	36.55	36.55 *	
Pressure (kPa)	3000 *	2565	2565	2765 *	2765 *	
Molar Flow (kgmole/h)	1292 *	1292	3.101e+004	3.101e+004	3.101e+004 *	
Mass Flow (kg/h)	4.742e+004	4.742e+004	1.138e+006	1.138e+006	1.138e+006	
Liquid Volume Flow (m3/h)	70.10	70.10	1682	1682	1682	
Heat Flow (kW)	-1.049e+005	-1.051e+005	-2.522e+006	-2.520e+006	-2.520e+006	
Name	Steam'	17	Flash out vapor	Flash out liquid	Hydrogen in	
Vapour Fraction	1.0000	0.8867	1.0000	0.0000	1.0000	
Temperature (C)	464.2	86.82	335.0	335.0	25.00 *	
Pressure (kPa)	2965 *	2565	2530	2530	2665 *	
Molar Flow (kgmole/h)	7000	4504	4357	147.0	3720	
Mass Flow (kg/h)	1.261e+005	1.285e+005	7.887e+004	4.968e+004	7500 *	
Liquid Volume Flow (m3/h)	126.4	267.5	205.5	62.01	107.4	
Heat Flow (kW)	-4.412e+005	-7.372e+004	-2.545e+004	-1.461e+004	-1.545	
Aspen Technology Inc. Aspen HYSYS Version 7.2 (24.0.0.7263) Page 1 of 25						

1	aspen NORWEGIAN UNIV OF Burlington, MA USA		Case Name: FERDIG2 RECYCLE.HSC				
2							
3							Unit Set: Oleekte
4							Date/Time: Tue Jun 12 09:00:31 2012
5							
6	Workbook: Case (Main) (continued)						
7							
8							
9							
10	Material Streams (continued)					Fluid Pkg:	All
11	Name	18	Flash in	19	C21+	C15-20	
12	Vapour Fraction	0.9674	0.9674	0.9448	0.0000	0.0000	
13	Temperature (C)	335.0 *	335.0 *	318.0	344.1 *	344.1 *	
14	Pressure (kPa)	2530	2530 *	2521	2521 *	2521 *	
15	Molar Flow (kgmole/h)	4504	4504 *	1538	13.73	42.91	
16	Mass Flow (kg/h)	1.285e+005	1.285e+005	1.285e+005	5806 *	1.092e+004 *	
17	Liquid Volume Flow (m3/h)	267.5	267.5	189.3	7.151	13.93	
18	Heat Flow (kW)	-4.007e+004	-4.007e+004	-5.397e+004	-1619	-3357	
19	Name	C10-14	C5-9	C1-4	CO2	iC5-9	
20	Vapour Fraction	0.0000	1.0000	1.0000	1.0000	1.0000	
21	Temperature (C)	344.1 *	344.1 *	344.1 *	344.1 *	344.1 *	
22	Pressure (kPa)	2521 *	2521 *	2521 *	2521 *	2521 *	
23	Molar Flow (kgmole/h)	134.4	211.0	105.6	142.1	34.35	
24	Mass Flow (kg/h)	2.289e+004 *	2.114e+004 *	4657 *	6253 *	3442 *	
25	Liquid Volume Flow (m3/h)	30.47	30.78	9.192	7.577	4.988	
26	Heat Flow (kW)	-7417	-6943	-2103	-1.501e+004	-1169	
27	Name	iC10+	CO	H2O	H2	19"	
28	Vapour Fraction	0.0000	1.0000	1.0000	1.0000	1.0000	
29	Temperature (C)	344.1 *	344.1 *	344.1 *	344.1 *	70.53	
30	Pressure (kPa)	2521 *	2521 *	2521 *	2521 *	2000	
31	Molar Flow (kgmole/h)	367.9	1.241	5.093	479.7	752.2	
32	Mass Flow (kg/h)	5.235e+004 *	34.76 *	91.76 *	967.1 *	1.386e+004	
33	Liquid Volume Flow (m3/h)	71.25	4.348e-002	9.194e-002	13.84	33.45	
34	Heat Flow (kW)	-1.721e+004	-34.86	-327.5	1229	-1.959e+004	
35	Name	19"	LPG	naphtha 2	naphtha	Fuel oil/diesel/kerosene	
36	Vapour Fraction	0.0000	1.0000	0.0000	0.0000	0.0000	
37	Temperature (C)	322.6	52.40	243.9	243.7	365.1	
38	Pressure (kPa)	2000	2000	2000	2000	2000	
39	Molar Flow (kgmole/h)	785.8	743.2	8.969	226.6	559.2	
40	Mass Flow (kg/h)	1.147e+005	1.296e+004	901.4	2.271e+004	9.198e+004	
41	Liquid Volume Flow (m3/h)	155.9	32.14	1.311	33.04	122.8	
42	Heat Flow (kW)	-4.019e+004	-1.929e+004	-405.7	-1.022e+004	-2.761e+004	
43	Name	19'	20	20'	5'	water	
44	Vapour Fraction	0.9572	1.0000	1.0000	1.0000	0.0000	
45	Temperature (C)	315.4	90.47	90.47 *	1030 *	19.09	
46	Pressure (kPa)	2100 *	3000 *	3000 *	2865 *	101.3 *	
47	Molar Flow (kgmole/h)	1538	743.2	743.2 *	3.629e+004 *	2.177e+004	
48	Mass Flow (kg/h)	1.285e+005	1.296e+004	1.296e+004	4.978e+005	3.922e+005 *	
49	Liquid Volume Flow (m3/h)	189.3	32.14	32.14	1080	393.0	
50	Heat Flow (kW)	-5.397e+004	-1.898e+004	-1.898e+004	-6.199e+005	-1.734e+006	
51	Name	HP water	Cooling water in 1	5*	HP steam*	5**	
52	Vapour Fraction	0.0000	0.0000	1.0000	0.0000	0.8051	
53	Temperature (C)	20.00 *	8.000 *	1030 *	20.00 *	30.00 *	
54	Pressure (kPa)	1.100e+004 *	101.3 *	2865 *	1.100e+004 *	2765 *	
55	Molar Flow (kgmole/h)	2.177e+004 *	2.514e+005	3.629e+004 *	2.177e+004	3.629e+004 *	
56	Mass Flow (kg/h)	3.922e+005	4.529e+006	4.978e+005	3.922e+005	4.978e+005	
57	Liquid Volume Flow (m3/h)	393.0	4538	1080	393.0	1080	
58	Heat Flow (kW)	-1.732e+006	-2.008e+007	-6.199e+005	-1.732e+006	-1.045e+006	
59	Name	HP steam**	5"	5"	5"	6"	
60	Vapour Fraction	1.0000	1.0000	1.0000	0.8777	0.8051	
61	Temperature (C)	510.0 *	864.4	462.8	121.8	30.00 *	
62	Pressure (kPa)	1.100e+004 *	2765	2765	2765	2765 *	
63	Molar Flow (kgmole/h)	2.177e+004	3.629e+004	3.629e+004	3.629e+004	3.629e+004 *	
64	Mass Flow (kg/h)	3.922e+005	4.978e+005	4.978e+005	4.978e+005	4.978e+005	
65	Liquid Volume Flow (m3/h)	393.0	1080	1080	1080	1080	
66	Heat Flow (kW)	-1.372e+006	-6.803e+005	-8.205e+005	-9.799e+005	-1.045e+006	
67							
68							
69							
70							
71	Aspen Technology Inc.		Aspen HYSYS Version 7.2 (24.0.0.7263)			Page 2 of 25	

aspen		NORWEGIAN UNIV OF Burlington, MA USA		Case Name: FERDIG2 RECYCLE.HSC		
				Unit Set: Oleekte		
				Date/Time: Tue Jun 12 09:00:31 2012		
Workbook: Case (Main) (continued)						
Material Streams (continued)				Fluid Pkg: All		
Name		Cooling water out 1	HP water'	HP steam'	HP steam	HP steam used 1
Vapour Fraction		0.0000	0.0000 *	1.0000 *	1.0000	1.0000
Temperature (C)		20.00 *	317.1	317.1	510.0 *	510.0
Pressure (kPa)		101.3	1.100e+004	1.100e+004	1.100e+004	1.100e+004
Molar Flow (kgmole/h)		2.514e+005	2.177e+004	2.177e+004	2.177e+004	7156
Mass Flow (kg/h)		4.529e+006	3.922e+005	3.922e+005	3.922e+005	1.289e+005
Liquid Volume Flow (m3/h)		4538	393.0	393.0	393.0	129.2
Heat Flow (kW)		-2.001e+007	-1.573e+006	-1.432e+006	-1.372e+006	-4.510e+005
Name		7*	8*	HPsteam used 1'	LP water in	LP water
Vapour Fraction		1.0000	1.0000	0.0000	0.0000	0.0000
Temperature (C)		30.45 *	210.0 *	40.45 *	19.92	20.00 *
Pressure (kPa)		2765 *	2665 *	1.100e+004	101.3 *	1000 *
Molar Flow (kgmole/h)		6.023e+004 *	6.023e+004 *	7156	2.839e+004	2.839e+004
Mass Flow (kg/h)		1.508e+006	1.508e+006	1.289e+005	5.115e+005	5.115e+005
Liquid Volume Flow (m3/h)		2634	2634	129.2	512.5	512.5
Heat Flow (kW)		-3.004e+006	-2.889e+006	-5.662e+005	-2.260e+006	-2.260e+006
Name		LP steam from FT re	9'	Cooling water in 2	10'	Cooling water out 2
Vapour Fraction		1.0000	1.0000	0.0000	0.7819	0.0000
Temperature (C)		190.0 *	210.0 *	8.000 *	30.00 *	18.00 *
Pressure (kPa)		1000	2665 *	101.3 *	2565 *	101.3
Molar Flow (kgmole/h)		2.839e+004	4.280e+004 *	9.665e+005	4.280e+004 *	9.665e+005
Mass Flow (kg/h)		5.115e+005	1.452e+006	1.741e+007	1.452e+006	1.741e+007
Liquid Volume Flow (m3/h)		512.5	2066	1.745e+004	2066	1.745e+004
Heat Flow (kW)		-1.867e+006	-3.258e+006	-7.720e+007	-3.467e+006	-7.699e+007
Name		HPsteamused	HPsteamused*	19'''	19'''	LPG*
Vapour Fraction		1.0000	1.0000	0.0000	0.0001	1.0000
Temperature (C)		510.0 *	332.0 *	315.4 *	322.6 *	70.53 *
Pressure (kPa)		1.100e+004 *	1.100e+004	2000 *	2000 *	2000 *
Molar Flow (kgmole/h)		364.5	364.5	785.8 *	785.8 *	743.2 *
Mass Flow (kg/h)		6566	6566	1.147e+005	1.147e+005	1.296e+004
Liquid Volume Flow (m3/h)		6.579	6.579	155.9	155.9	32.14
Heat Flow (kW)		-2.297e+004	-2.388e+004	-4.110e+004	-4.019e+004	-1.914e+004
Name		Cooling water used	LPG**	Cooling water used*	naphtha*	Coolingwater in
Vapour Fraction		0.0000	1.0000	0.0000	1.0000	0.0000
Temperature (C)		8.000 *	52.40 *	18.00 *	322.6 *	8.000 *
Pressure (kPa)		101.3 *	2000 *	101.3	2000 *	101.3 *
Molar Flow (kgmole/h)		714.5	743.2 *	714.5	226.6 *	1.106e+004
Mass Flow (kg/h)		1.287e+004	1.296e+004	1.287e+004	2.271e+004	1.992e+005
Liquid Volume Flow (m3/h)		12.90	32.14	12.90	33.04	199.6
Heat Flow (kW)		-5.707e+004	-1.929e+004	-5.691e+004	-7834	-8.833e+005
Name		naphtha**	Coolingwater out	19''	Cooling water in	Cooling water out
Vapour Fraction		0.0000	0.0000	1.0000	0.0000	0.0000
Temperature (C)		243.7 *	18.00 *	315.4 *	8.000 *	18.00 *
Pressure (kPa)		2000 *	101.3	2000 *	101.3 *	101.3
Molar Flow (kgmole/h)		226.6 *	1.106e+004	752.2 *	1.138e+004	1.138e+004
Mass Flow (kg/h)		2.271e+004	1.992e+005	1.386e+004	2.050e+005	2.050e+005
Liquid Volume Flow (m3/h)		33.04	199.6	33.45	205.4	205.4
Heat Flow (kW)		-1.022e+004	-8.809e+005	-1.713e+004	-9.089e+005	-9.064e+005
Name		19'''	naphtha2*	HPSteam used*	naphtha2**	HPSteam used
Vapour Fraction		1.0000	0.0000	0.0000	0.0000	1.0000
Temperature (C)		70.53 *	70.53 *	81.00 *	243.9 *	510.0 *
Pressure (kPa)		2000 *	2000 *	1.100e+004	2000 *	1.100e+004 *
Molar Flow (kgmole/h)		752.2 *	8.969 *	8.457	8.969 *	8.457
Mass Flow (kg/h)		1.386e+004	901.4	152.4	901.4	152.4
Liquid Volume Flow (m3/h)		33.45	1.311	0.1527	1.311	0.1527
Heat Flow (kW)		-1.959e+004	-534.4	-661.7	-405.7	-533.0
Aspen Technology Inc. Aspen HYSYS Version 7.2 (24.0.0.7263) Page 3 of 25						

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Material Streams (continued)

Fluid Pkg: All

Name	Fueloil/diesel/kerosene	HP steam in	Fueloil/diesel/kerosene	HP steam out	
Vapour Fraction	0.0000	1.0000	0.0001	1.0000	
Temperature (C)	322.6 *	510.0 *	365.1 *	333.0 *	
Pressure (kPa)	2000 *	1.100e+004 *	2000 *	1.100e+004 *	
Molar Flow (kgmole/h)	559.2 *	1741	559.2 *	1741	
Mass Flow (kg/h)	9.198e+004	3.136e+004	9.198e+004	3.136e+004	
Liquid Volume Flow (m3/h)	122.8	31.43	122.8	31.43	
Heat Flow (kW)	-3.193e+004	-1.097e+005	-2.761e+004	-1.140e+005	

Compositions

Fluid Pkg: All

Name	Natural Gas	Natural Gas'	1	2	3	
Master Comp Mass Frac (Methane)	0.8736 *	0.8736	0.6331	0.6331		0.4603
Master Comp Mass Frac (Ethane)	0.0345 *	0.0345	0.0296	0.0296		0.0001
Master Comp Mass Frac (Propane)	0.0379 *	0.0379	0.0550	0.0550		0.0000
Master Comp Mass Frac (i-Butane)	0.0333 *	0.0333	0.0234	0.0234		0.0000
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000	0.0040	0.0040		0.0000
Master Comp Mass Frac (i-Pentane)	0.0207 *	0.0207	0.0146	0.0146		0.0000
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000	0.0021	0.0021		0.0000
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000	0.0009	0.0009		0.0000
Master Comp Mass Frac (n-Heptane)	0.0000 *	0.0000	0.0040	0.0040		0.0000
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000	0.0001	0.0001		0.0000
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000	0.0001	0.0001		0.0000
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (H2O)	0.0000 *	0.0000	0.0007	0.0007		0.3353
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000	0.0053	0.0053		0.0062
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000	0.0000	0.0000		0.0000
Master Comp Mass Frac (CO)	0.0000 *	0.0000	0.0055	0.0055		0.0028
Master Comp Mass Frac (CO2)	0.0000 *	0.0000	0.2205	0.2205		0.1946
Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0000	0.0011	0.0011		0.0007
Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000	0.0000	0.0000		0.0000

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1	aspen NORWEGIAN UNIV OF Burlington, MA USA		Case Name: FERDIG2 RECYCLE.HSC				
2			Unit Set: Oleekte				
3			Date/Time: Tue Jun 12 09:00:31 2012				
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5	Workbook: Case (Main) (continued)						
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10	Compositions (continued)					Fluid Pkg:	All
11	Name	liq	Steam	4	5	liq2	
12	Master Comp Mass Frac (Methane)	0.4603	0.0000 *	0.4603	0.0121	0.0121	
13	Master Comp Mass Frac (Ethane)	0.0001	0.0000 *	0.0001	0.0001	0.0001	
14	Master Comp Mass Frac (Propane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
15	Master Comp Mass Frac (i-Butane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
16	Master Comp Mass Frac (n-Butane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
17	Master Comp Mass Frac (i-Pentane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
18	Master Comp Mass Frac (n-Pentane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
19	Master Comp Mass Frac (n-Hexane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
20	Master Comp Mass Frac (n-Heptane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
21	Master Comp Mass Frac (n-Octane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
22	Master Comp Mass Frac (n-Nonane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
23	Master Comp Mass Frac (n-Decane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
24	Master Comp Mass Frac (n-C11)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
25	Master Comp Mass Frac (n-C12)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
26	Master Comp Mass Frac (n-C13)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
27	Master Comp Mass Frac (n-C14)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
28	Master Comp Mass Frac (n-C15)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
29	Master Comp Mass Frac (n-C16)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
30	Master Comp Mass Frac (n-C17)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
31	Master Comp Mass Frac (n-C18)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
32	Master Comp Mass Frac (n-C19)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
33	Master Comp Mass Frac (n-C20)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
34	Master Comp Mass Frac (n-C30)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
35	Master Comp Mass Frac (Oxygen)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
36	Master Comp Mass Frac (H2O)	0.3353	1.0000 *	0.3353	0.2577	0.2577	
37	Master Comp Mass Frac (Hydrogen)	0.0062	0.0000 *	0.0062	0.0738	0.0738	
38	Master Comp Mass Frac (Nitrogen)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
39	Master Comp Mass Frac (CO)	0.0028	0.0000 *	0.0028	0.4896	0.4896	
40	Master Comp Mass Frac (CO2)	0.1946	0.0000 *	0.1946	0.1663	0.1663	
41	Master Comp Mass Frac (3-Mhexane)	0.0007	0.0000 *	0.0007	0.0004	0.0004	
42	Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000 *	0.0000	0.0000	0.0000	
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71	Aspen Technology Inc.		Aspen HYSYS Version 7.2 (24.0.0.7263)			Page 5 of 25	

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	Oxygen in	6	7	Water out 1	8
Master Comp Mass Frac (Methane)	0.0000 *	0.0121	0.0162	0.0000	0.0636
Master Comp Mass Frac (Ethane)	0.0000 *	0.0001	0.0001	0.0000	0.0172
Master Comp Mass Frac (Propane)	0.0000 *	0.0000	0.0000	0.0000	0.0178
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000	0.0000	0.0000	0.0129
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000	0.0000	0.0000	0.0068
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000	0.0000	0.0000	0.0030
Master Comp Mass Frac (n-Heptane)	0.0000 *	0.0000	0.0000	0.0000	0.0012
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000	0.0000	0.0000	0.0005
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000	0.0000	0.0000	0.0002
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000	0.0000	0.0000	0.0001
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Oxygen)	1.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (H2O)	0.0000 *	0.2577	0.0026	0.9983	0.0015
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0738	0.0992	0.0000	0.0261
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO)	0.0000 *	0.4896	0.6582	0.0000	0.1789
Master Comp Mass Frac (CO2)	0.0000 *	0.1663	0.2231	0.0017	0.6701
Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0004	0.0006	0.0000	0.0002
Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000	0.0000	0.0000	0.0000

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	9	Wax	10	11	Light HC
Master Comp Mass Frac (Methane)	0.0670	0.0006	0.0670	0.0790	0.0034
Master Comp Mass Frac (Ethane)	0.0195	0.0003	0.0195	0.0228	0.0044
Master Comp Mass Frac (Propane)	0.0206	0.0006	0.0206	0.0236	0.0142
Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Butane)	0.0159	0.0008	0.0159	0.0171	0.0319
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Pentane)	0.0099	0.0008	0.0099	0.0091	0.0497
Master Comp Mass Frac (n-Hexane)	0.0061	0.0008	0.0061	0.0040	0.0616
Master Comp Mass Frac (n-Heptane)	0.0044	0.0009	0.0044	0.0016	0.0680
Master Comp Mass Frac (n-Octane)	0.0037	0.0012	0.0037	0.0006	0.0710
Master Comp Mass Frac (n-Nonane)	0.0034	0.0017	0.0034	0.0002	0.0718
Master Comp Mass Frac (n-Decane)	0.0032	0.0026	0.0032	0.0001	0.0711
Master Comp Mass Frac (n-C11)	0.0031	0.0038	0.0031	0.0000	0.0693
Master Comp Mass Frac (n-C12)	0.0030	0.0056	0.0030	0.0000	0.0664
Master Comp Mass Frac (n-C13)	0.0028	0.0083	0.0028	0.0000	0.0622
Master Comp Mass Frac (n-C14)	0.0025	0.0123	0.0025	0.0000	0.0565
Master Comp Mass Frac (n-C15)	0.0023	0.0159	0.0023	0.0000	0.0509
Master Comp Mass Frac (n-C16)	0.0020	0.0204	0.0020	0.0000	0.0443
Master Comp Mass Frac (n-C17)	0.0016	0.0257	0.0016	0.0000	0.0370
Master Comp Mass Frac (n-C18)	0.0013	0.0306	0.0013	0.0000	0.0299
Master Comp Mass Frac (n-C19)	0.0011	0.0344	0.0011	0.0000	0.0238
Master Comp Mass Frac (n-C20)	0.0007	0.0400	0.0007	0.0000	0.0161
Master Comp Mass Frac (n-C30)	0.0002	0.7826	0.0002	0.0000	0.0037
Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (H2O)	0.1085	0.0015	0.1085	0.0011	0.0001
Master Comp Mass Frac (Hydrogen)	0.0019	0.0000	0.0019	0.0023	0.0000
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO)	0.0195	0.0001	0.0195	0.0230	0.0004
Master Comp Mass Frac (CO2)	0.6957	0.0087	0.6957	0.8155	0.0890
Master Comp Mass Frac (3-Mhexane)	0.0002	0.0000	0.0002	0.0001	0.0032
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000	0.0000	0.0000	0.0000

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	Water out 2	Purge	7	12	16
Master Comp Mass Frac (Methane)	0.0000	0.0790	0.0636	0.0790	0.0790
Master Comp Mass Frac (Ethane)	0.0000	0.0228	0.0172	0.0228	0.0228
Master Comp Mass Frac (Propane)	0.0000	0.0236	0.0178	0.0236	0.0236
Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Butane)	0.0000	0.0171	0.0129	0.0171	0.0171
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000	0.0091	0.0068	0.0091	0.0091
Master Comp Mass Frac (n-Hexane)	0.0000	0.0040	0.0030	0.0040	0.0040
Master Comp Mass Frac (n-Heptane)	0.0000	0.0016	0.0012	0.0016	0.0016
Master Comp Mass Frac (n-Octane)	0.0000	0.0006	0.0005	0.0006	0.0006
Master Comp Mass Frac (n-Nonane)	0.0000	0.0002	0.0002	0.0002	0.0002
Master Comp Mass Frac (n-Decane)	0.0000	0.0001	0.0001	0.0001	0.0001
Master Comp Mass Frac (n-C11)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C12)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C13)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C14)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C15)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C16)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C17)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C18)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C19)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C20)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C30)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (H2O)	0.9836	0.0011	0.0015	0.0011	0.0011
Master Comp Mass Frac (Hydrogen)	0.0000	0.0023	0.0261	0.0023	0.0023
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO)	0.0000	0.0230	0.1789	0.0230	0.0230
Master Comp Mass Frac (CO2)	0.0164	0.8155	0.6701	0.8155	0.8155
Master Comp Mass Frac (3-Mhexane)	0.0000	0.0001	0.0002	0.0001	0.0001
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000	0.0000	0.0000	0.0000

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	16'	15	13	14	14'
Master Comp Mass Frac (Methane)	0.0790 *	0.0790	0.0790	0.0790	0.0790 *
Master Comp Mass Frac (Ethane)	0.0228 *	0.0228	0.0228	0.0228	0.0228 *
Master Comp Mass Frac (Propane)	0.0236 *	0.0236	0.0236	0.0236	0.0236 *
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-Butane)	0.0171 *	0.0171	0.0171	0.0171	0.0171 *
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-Pentane)	0.0091 *	0.0091	0.0091	0.0091	0.0091 *
Master Comp Mass Frac (n-Hexane)	0.0040 *	0.0040	0.0040	0.0040	0.0040 *
Master Comp Mass Frac (n-Heptane)	0.0016 *	0.0016	0.0016	0.0016	0.0016 *
Master Comp Mass Frac (n-Octane)	0.0006 *	0.0006	0.0006	0.0006	0.0006 *
Master Comp Mass Frac (n-Nonane)	0.0002 *	0.0002	0.0002	0.0002	0.0002 *
Master Comp Mass Frac (n-Decane)	0.0001 *	0.0001	0.0001	0.0001	0.0001 *
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (H2O)	0.0011 *	0.0011	0.0011	0.0011	0.0011 *
Master Comp Mass Frac (Hydrogen)	0.0023 *	0.0023	0.0023	0.0023	0.0023 *
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (CO)	0.0230 *	0.0230	0.0230	0.0230	0.0230 *
Master Comp Mass Frac (CO2)	0.8155 *	0.8155	0.8155	0.8155	0.8155 *
Master Comp Mass Frac (3-Mhexane)	0.0001 *	0.0001	0.0001	0.0001	0.0001 *
Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000	0.0000	0.0000	0.0000 *

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	Steam'	17	Flash out vapor	Flash out liquid	Hydrogen in
Master Comp Mass Frac (Methane)	0.0000	0.0020	0.0032	0.0000	0.0000 *
Master Comp Mass Frac (Ethane)	0.0000	0.0024	0.0039	0.0000	0.0000 *
Master Comp Mass Frac (Propane)	0.0000	0.0074	0.0120	0.0001	0.0000 *
Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-Butane)	0.0000	0.0164	0.0265	0.0004	0.0000 *
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (n-Pentane)	0.0000	0.0254	0.0409	0.0008	0.0000 *
Master Comp Mass Frac (n-Hexane)	0.0000	0.0314	0.0503	0.0013	0.0000 *
Master Comp Mass Frac (n-Heptane)	0.0000	0.0346	0.0552	0.0020	0.0000 *
Master Comp Mass Frac (n-Octane)	0.0000	0.0362	0.0573	0.0028	0.0000 *
Master Comp Mass Frac (n-Nonane)	0.0000	0.0369	0.0578	0.0037	0.0000 *
Master Comp Mass Frac (n-Decane)	0.0000	0.0369	0.0571	0.0049	0.0000 *
Master Comp Mass Frac (n-C11)	0.0000	0.0366	0.0556	0.0062	0.0000 *
Master Comp Mass Frac (n-C12)	0.0000	0.0359	0.0534	0.0079	0.0000 *
Master Comp Mass Frac (n-C13)	0.0000	0.0349	0.0507	0.0099	0.0000 *
Master Comp Mass Frac (n-C14)	0.0000	0.0338	0.0473	0.0124	0.0000 *
Master Comp Mass Frac (n-C15)	0.0000	0.0326	0.0439	0.0146	0.0000 *
Master Comp Mass Frac (n-C16)	0.0000	0.0313	0.0404	0.0169	0.0000 *
Master Comp Mass Frac (n-C17)	0.0000	0.0299	0.0360	0.0201	0.0000 *
Master Comp Mass Frac (n-C18)	0.0000	0.0285	0.0319	0.0231	0.0000 *
Master Comp Mass Frac (n-C19)	0.0000	0.0270	0.0279	0.0257	0.0000 *
Master Comp Mass Frac (n-C20)	0.0000	0.0256	0.0238	0.0285	0.0000 *
Master Comp Mass Frac (n-C30)	0.0000	0.3448	0.0469	0.8177	0.0000 *
Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (H2O)	1.0000	0.0007	0.0012	0.0000	0.0000 *
Master Comp Mass Frac (Hydrogen)	0.0000	0.0584	0.0949	0.0003	1.0000 *
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Master Comp Mass Frac (CO)	0.0000	0.0003	0.0004	0.0000	0.0000 *
Master Comp Mass Frac (CO2)	0.0000	0.0486	0.0790	0.0005	0.0000 *
Master Comp Mass Frac (3-Mhexane)	0.0000	0.0016	0.0026	0.0001	0.0000 *
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000	0.0000	0.0000	0.0000 *

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	18	Flash in	19	C21+	C15-20
Master Comp Mass Frac (Methane)	0.0020	0.0020 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Ethane)	0.0024	0.0024 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Propane)	0.0074	0.0074 *	0.0362	0.0000 *	0.0000 *
Master Comp Mass Frac (i-Butane)	0.0000	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Butane)	0.0164	0.0164 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Pentane)	0.0254	0.0254 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Hexane)	0.0314	0.0314 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Heptane)	0.0346	0.0346 *	0.1644	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Octane)	0.0362	0.0362 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Nonane)	0.0369	0.0369 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Decane)	0.0369	0.0369 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C11)	0.0366	0.0366 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C12)	0.0359	0.0359 *	0.1780	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C13)	0.0349	0.0349 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C14)	0.0338	0.0338 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C15)	0.0326	0.0326 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C16)	0.0313	0.0313 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C17)	0.0299	0.0299 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C18)	0.0285	0.0285 *	0.0849	0.0000 *	1.0000 *
Master Comp Mass Frac (n-C19)	0.0270	0.0270 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C20)	0.0256	0.0256 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C30)	0.3448	0.3448 *	0.0452	1.0000 *	0.0000 *
Master Comp Mass Frac (Oxygen)	0.0000	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (H2O)	0.0007	0.0007 *	0.0007	0.0000 *	0.0000 *
Master Comp Mass Frac (Hydrogen)	0.0584	0.0584 *	0.0075	0.0000 *	0.0000 *
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (CO)	0.0003	0.0003 *	0.0003	0.0000 *	0.0000 *
Master Comp Mass Frac (CO2)	0.0486	0.0486 *	0.0486	0.0000 *	0.0000 *
Master Comp Mass Frac (3-Mhexane)	0.0016	0.0016 *	0.0268	0.0000 *	0.0000 *
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000 *	0.4072	0.0000 *	0.0000 *

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1	<div><div>aspen</div><div>NORWEGIAN UNIV OF Burlington, MA USA</div></div>		Case Name: FERDIG2 RECYCLE.HSC			
2			Unit Set: Oleekte			
3			Date/Time: Tue Jun 12 09:00:31 2012			
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7	Workbook: Case (Main) (continued)					
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10	Compositions (continued)			Fluid Pkg:	All	
11	Name	C10-14	C5-9	C1-4	CO2	iC5-9
12	Master Comp Mass Frac (Methane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
13	Master Comp Mass Frac (Ethane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
14	Master Comp Mass Frac (Propane)	0.0000 *	0.0000 *	1.0000 *	0.0000 *	0.0000 *
15	Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
16	Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
17	Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
18	Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
19	Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
20	Master Comp Mass Frac (n-Heptane)	0.0000 *	1.0000 *	0.0000 *	0.0000 *	0.0000 *
21	Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
22	Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
23	Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
24	Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
25	Master Comp Mass Frac (n-C12)	1.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
26	Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
27	Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
28	Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
29	Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
30	Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
31	Master Comp Mass Frac (n-C18)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
32	Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
33	Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
34	Master Comp Mass Frac (n-C30)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
35	Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
36	Master Comp Mass Frac (H2O)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
37	Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
38	Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
39	Master Comp Mass Frac (CO)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
40	Master Comp Mass Frac (CO2)	0.0000 *	0.0000 *	0.0000 *	1.0000 *	0.0000 *
41	Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	1.0000 *
42	Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	IC10+	CO	H2O	H2	19"
Master Comp Mass Frac (Methane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (Ethane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (Propane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.3357
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Heptane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.1077
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (H2O)	0.0000 *	0.0000 *	1.0000 *	0.0000 *	0.0066
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000 *	0.0000 *	1.0000 *	0.0698
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (CO)	0.0000 *	1.0000 *	0.0000 *	0.0000 *	0.0025
Master Comp Mass Frac (CO2)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.4511
Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0258
Master Comp Mass Frac (4-Mnonane)	1.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0008

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	19"	LPG	naphtha 2	naphtha	Fuel oil/diesel/keros
Master Comp Mass Frac (Methane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Ethane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Propane)	0.0000	0.3590	0.0004	0.0002	0.0000
Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Hexane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Heptane)	0.1713	0.0575	0.8300	0.8628	0.0006
Master Comp Mass Frac (n-Octane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Nonane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Decane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C11)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C12)	0.1996	0.0000	0.0000	0.0000	0.2488
Master Comp Mass Frac (n-C13)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C14)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C15)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C16)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C17)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C18)	0.0952	0.0000	0.0000	0.0000	0.1187
Master Comp Mass Frac (n-C19)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C20)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C30)	0.0506	0.0000	0.0000	0.0000	0.0631
Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (H2O)	0.0000	0.0071	0.0000	0.0000	0.0000
Master Comp Mass Frac (Hydrogen)	0.0000	0.0746	0.0000	0.0000	0.0000
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO)	0.0000	0.0027	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO2)	0.0000	0.4825	0.0000	0.0000	0.0000
Master Comp Mass Frac (3-Mhexane)	0.0269	0.0167	0.1577	0.1357	0.0000
Master Comp Mass Frac (4-Mnonane)	0.4564	0.0000	0.0118	0.0014	0.5687

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Aspen HYSYS Version 7.2 (24.0.0.7263)

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1				Case Name: FERDIG2 RECYCLE.HSC		
2	aspen	NORWEGIAN UNIV OF Burlington, MA USA	Unit Set: Oleekte			
3			Date/Time: Tue Jun 12 09:00:31 2012			
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7	Workbook: Case (Main) (continued)					
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10	Compositions (continued)				Fluid Pkg: All	
11	Name	19'	20	20'	5'	water
12	Master Comp Mass Frac (Methane)	0.0000	0.0000	0.0000 *	0.0121 *	0.0000 *
13	Master Comp Mass Frac (Ethane)	0.0000	0.0000	0.0000 *	0.0001 *	0.0000 *
14	Master Comp Mass Frac (Propane)	0.0362	0.3590	0.3590 *	0.0000 *	0.0000 *
15	Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
16	Master Comp Mass Frac (n-Butane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
17	Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
18	Master Comp Mass Frac (n-Pentane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
19	Master Comp Mass Frac (n-Hexane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
20	Master Comp Mass Frac (n-Heptane)	0.1644	0.0575	0.0575 *	0.0000 *	0.0000 *
21	Master Comp Mass Frac (n-Octane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
22	Master Comp Mass Frac (n-Nonane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
23	Master Comp Mass Frac (n-Decane)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
24	Master Comp Mass Frac (n-C11)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
25	Master Comp Mass Frac (n-C12)	0.1780	0.0000	0.0000 *	0.0000 *	0.0000 *
26	Master Comp Mass Frac (n-C13)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
27	Master Comp Mass Frac (n-C14)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
28	Master Comp Mass Frac (n-C15)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
29	Master Comp Mass Frac (n-C16)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
30	Master Comp Mass Frac (n-C17)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
31	Master Comp Mass Frac (n-C18)	0.0849	0.0000	0.0000 *	0.0000 *	0.0000 *
32	Master Comp Mass Frac (n-C19)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
33	Master Comp Mass Frac (n-C20)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
34	Master Comp Mass Frac (n-C30)	0.0452	0.0000	0.0000 *	0.0000 *	0.0000 *
35	Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
36	Master Comp Mass Frac (H2O)	0.0007	0.0071	0.0071 *	0.2577 *	1.0000 *
37	Master Comp Mass Frac (Hydrogen)	0.0075	0.0746	0.0746 *	0.0738 *	0.0000 *
38	Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000 *	0.0000 *	0.0000 *
39	Master Comp Mass Frac (CO)	0.0003	0.0027	0.0027 *	0.4896 *	0.0000 *
40	Master Comp Mass Frac (CO2)	0.0486	0.4825	0.4825 *	0.1663 *	0.0000 *
41	Master Comp Mass Frac (3-Mhexane)	0.0268	0.0167	0.0167 *	0.0004 *	0.0000 *
42	Master Comp Mass Frac (4-Mnonane)	0.4072	0.0000	0.0000 *	0.0000 *	0.0000 *
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71	Aspen Technology Inc		Aspen HYSYS Version 7.2 (24 0.0.7263)		Page 15 of 25	

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NORWEGIAN UNIV OF

Burlington, MA

USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	HP water	Cooling water in 1	5*	HP steam*	5**
Master Comp Mass Frac (Methane)	0.0000 *	0.0000 *	0.0121 *	0.0000 *	0.0121 *
Master Comp Mass Frac (Ethane)	0.0000 *	0.0000 *	0.0001 *	0.0000 *	0.0000 *
Master Comp Mass Frac (Propane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Heptane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (H2O)	1.0000 *	1.0000 *	0.2577 *	1.0000 *	0.2577 *
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000 *	0.0738 *	0.0000 *	0.0738 *
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *
Master Comp Mass Frac (CO)	0.0000 *	0.0000 *	0.4896 *	0.0000 *	0.4896 *
Master Comp Mass Frac (CO2)	0.0000 *	0.0000 *	0.1663 *	0.0000 *	0.1663 *
Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0000 *	0.0004 *	0.0000 *	0.0004 *
Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000 *	0.0000 *	0.0000 *	0.0000 *

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	HP steam**	5"	5"	5"	6"
Master Comp Mass Frac (Methane)	0.0000	0.0121	0.0121	0.0121	0.0121
Master Comp Mass Frac (Ethane)	0.0000	0.0001	0.0001	0.0001	0.0001
Master Comp Mass Frac (Propane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Hexane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Heptane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Octane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Nonane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Decane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C11)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C12)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C13)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C14)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C15)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C16)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C17)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C18)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C19)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C20)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C30)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (H2O)	1.0000	0.2577	0.2577	0.2577	0.2577
Master Comp Mass Frac (Hydrogen)	0.0000	0.0738	0.0738	0.0738	0.0738
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO)	0.0000	0.4896	0.4896	0.4896	0.4896
Master Comp Mass Frac (CO2)	0.0000	0.1663	0.1663	0.1663	0.1663
Master Comp Mass Frac (3-Mhexane)	0.0000	0.0004	0.0004	0.0004	0.0004
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000	0.0000	0.0000	0.0000

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	Cooling water out 1	HP water'	HP steam'	HP steam	HP steam used 1
Master Comp Mass Frac (Methane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Ethane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Propane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (i-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Butane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Hexane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Heptane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Octane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Nonane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-Decane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C11)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C12)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C13)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C14)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C15)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C16)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C17)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C18)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C19)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C20)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (n-C30)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (H2O)	1.0000	1.0000	1.0000	1.0000	1.0000
Master Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (CO2)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (3-Mhexane)	0.0000	0.0000	0.0000	0.0000	0.0000
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000	0.0000	0.0000	0.0000

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	7*	8*	HPsteam used 1'	LP water in	LP water
Master Comp Mass Frac (Methane)	0.0636 *	0.0636 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (Ethane)	0.0172 *	0.0172 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (Propane)	0.0178 *	0.0178 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Butane)	0.0129 *	0.0129 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Pentane)	0.0068 *	0.0068 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Hexane)	0.0030 *	0.0030 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Heptane)	0.0012 *	0.0012 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Octane)	0.0005 *	0.0005 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Nonane)	0.0002 *	0.0002 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-Decane)	0.0001 *	0.0001 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (H2O)	0.0015 *	0.0015 *	1.0000	1.0000 *	1.0000
Master Comp Mass Frac (Hydrogen)	0.0261 *	0.0261 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (CO)	0.1789 *	0.1789 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (CO2)	0.6701 *	0.6701 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (3-Mhexane)	0.0002 *	0.0002 *	0.0000	0.0000 *	0.0000
Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000

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NORWEGIAN UNIV OF

Burlington, MA

USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	LP steam from FT re	g'	Cooling water in 2	10'	Cooling water out 2
Master Comp Mass Frac (Methane)	0.0000	0.0670 *	0.0000 *	0.0670 *	0.0000
Master Comp Mass Frac (Ethane)	0.0000	0.0195 *	0.0000 *	0.0195 *	0.0000
Master Comp Mass Frac (Propane)	0.0000	0.0206 *	0.0000 *	0.0206 *	0.0000
Master Comp Mass Frac (i-Butane)	0.0000	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Butane)	0.0000	0.0159 *	0.0000 *	0.0159 *	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000	0.0099 *	0.0000 *	0.0099 *	0.0000
Master Comp Mass Frac (n-Hexane)	0.0000	0.0061 *	0.0000 *	0.0061 *	0.0000
Master Comp Mass Frac (n-Heptane)	0.0000	0.0044 *	0.0000 *	0.0044 *	0.0000
Master Comp Mass Frac (n-Octane)	0.0000	0.0037 *	0.0000 *	0.0037 *	0.0000
Master Comp Mass Frac (n-Nonane)	0.0000	0.0034 *	0.0000 *	0.0034 *	0.0000
Master Comp Mass Frac (n-Decane)	0.0000	0.0032 *	0.0000 *	0.0032 *	0.0000
Master Comp Mass Frac (n-C11)	0.0000	0.0031 *	0.0000 *	0.0031 *	0.0000
Master Comp Mass Frac (n-C12)	0.0000	0.0030 *	0.0000 *	0.0030 *	0.0000
Master Comp Mass Frac (n-C13)	0.0000	0.0028 *	0.0000 *	0.0028 *	0.0000
Master Comp Mass Frac (n-C14)	0.0000	0.0025 *	0.0000 *	0.0025 *	0.0000
Master Comp Mass Frac (n-C15)	0.0000	0.0023 *	0.0000 *	0.0023 *	0.0000
Master Comp Mass Frac (n-C16)	0.0000	0.0020 *	0.0000 *	0.0020 *	0.0000
Master Comp Mass Frac (n-C17)	0.0000	0.0016 *	0.0000 *	0.0016 *	0.0000
Master Comp Mass Frac (n-C18)	0.0000	0.0013 *	0.0000 *	0.0013 *	0.0000
Master Comp Mass Frac (n-C19)	0.0000	0.0011 *	0.0000 *	0.0011 *	0.0000
Master Comp Mass Frac (n-C20)	0.0000	0.0007 *	0.0000 *	0.0007 *	0.0000
Master Comp Mass Frac (n-C30)	0.0000	0.0002 *	0.0000 *	0.0002 *	0.0000
Master Comp Mass Frac (Oxygen)	0.0000	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (H2O)	1.0000	0.1085 *	1.0000 *	0.1085 *	1.0000
Master Comp Mass Frac (Hydrogen)	0.0000	0.0019 *	0.0000 *	0.0019 *	0.0000
Master Comp Mass Frac (Nitrogen)	0.0000	0.0000 *	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (CO)	0.0000	0.0195 *	0.0000 *	0.0195 *	0.0000
Master Comp Mass Frac (CO2)	0.0000	0.6957 *	0.0000 *	0.6957 *	0.0000
Master Comp Mass Frac (3-Mhexane)	0.0000	0.0002 *	0.0000 *	0.0002 *	0.0000
Master Comp Mass Frac (4-Mnonane)	0.0000	0.0000 *	0.0000 *	0.0000 *	0.0000

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Aspen HYSYS Version 7.2 (24.0.0.7263)

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1	aspen	NORWEGIAN UNIV OF Burlington, MA USA	Case Name: FERDIG2 RECYCLE.HSC			
2			Unit Set: Oleekte			
3			Date/Time: Tue Jun 12 09:00:31 2012			
4						
5	Workbook: Case (Main) (continued)					
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10	Compositions (continued)				Fluid Pkg:	All
11	Name	HPsteamused	HPsteamused*	19***	19***	LPG*
12	Master Comp Mass Frac (Methane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
13	Master Comp Mass Frac (Ethane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
14	Master Comp Mass Frac (Propane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.3590 *
15	Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
16	Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
17	Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
18	Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
19	Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
20	Master Comp Mass Frac (n-Heptane)	0.0000 *	0.0000	0.1713 *	0.1713 *	0.0575 *
21	Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
22	Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
23	Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
24	Master Comp Mass Frac (n-C11)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
25	Master Comp Mass Frac (n-C12)	0.0000 *	0.0000	0.1996 *	0.1996 *	0.0000 *
26	Master Comp Mass Frac (n-C13)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
27	Master Comp Mass Frac (n-C14)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
28	Master Comp Mass Frac (n-C15)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
29	Master Comp Mass Frac (n-C16)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
30	Master Comp Mass Frac (n-C17)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
31	Master Comp Mass Frac (n-C18)	0.0000 *	0.0000	0.0952 *	0.0952 *	0.0000 *
32	Master Comp Mass Frac (n-C19)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
33	Master Comp Mass Frac (n-C20)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
34	Master Comp Mass Frac (n-C30)	0.0000 *	0.0000	0.0506 *	0.0506 *	0.0000 *
35	Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
36	Master Comp Mass Frac (H2O)	1.0000 *	1.0000	0.0000 *	0.0000 *	0.0071 *
37	Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0746 *
38	Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000 *
39	Master Comp Mass Frac (CO)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0027 *
40	Master Comp Mass Frac (CO2)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.4825 *
41	Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0000	0.0269 *	0.0269 *	0.0167 *
42	Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000	0.4564 *	0.4564 *	0.0000 *
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71	Aspen Technology Inc.		Aspen HYSYS Version 7.2 (24.0.0.7263)		Page 21 of 25	
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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	Cooling water used	LPG**	Cooling water used*	naphtha*	Coolingwater in
Master Comp Mass Frac (Methane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Ethane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Propane)	0.0000 *	0.3590 *	0.0000	0.0002 *	0.0000 *
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Heptane)	0.0000 *	0.0575 *	0.0000	0.8628 *	0.0000 *
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (H2O)	1.0000 *	0.0071 *	1.0000	0.0000 *	1.0000 *
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0746 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (CO)	0.0000 *	0.0027 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (CO2)	0.0000 *	0.4825 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0167 *	0.0000	0.1357 *	0.0000 *
Master Comp Mass Frac (4-Mnonane)	0.0000 *	0.0000 *	0.0000	0.0014 *	0.0000 *

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NORWEGIAN UNIV OF

Burlington, MA

USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	naphtha**	Coolingwater out	19**	Cooling water in	Cooling water out
Master Comp Mass Frac (Methane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (Ethane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (Propane)	0.0002 *	0.0000	0.3357 *	0.0000 *	0.0000
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Heptane)	0.8628 *	0.0000	0.1077 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (H2O)	0.0000 *	1.0000	0.0066 *	1.0000 *	1.0000
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000	0.0698 *	0.0000 *	0.0000
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000	0.0000 *	0.0000 *	0.0000
Master Comp Mass Frac (CO)	0.0000 *	0.0000	0.0025 *	0.0000 *	0.0000
Master Comp Mass Frac (CO2)	0.0000 *	0.0000	0.4511 *	0.0000 *	0.0000
Master Comp Mass Frac (3-Mhexane)	0.1357 *	0.0000	0.0258 *	0.0000 *	0.0000
Master Comp Mass Frac (4-Mnonane)	0.0014 *	0.0000	0.0008 *	0.0000 *	0.0000

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)

Fluid Pkg: All

Name	19***	naphtha2*	HPSteam used*	naphtha2**	HPSteam used
Master Comp Mass Frac (Methane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Ethane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Propane)	0.3357 *	0.0004 *	0.0000	0.0004 *	0.0000 *
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Heptane)	0.1077 *	0.8300 *	0.0000	0.8300 *	0.0000 *
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C12)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C18)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (n-C30)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (H2O)	0.0066 *	0.0000 *	1.0000	0.0000 *	1.0000 *
Master Comp Mass Frac (Hydrogen)	0.0698 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (CO)	0.0025 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (CO2)	0.4511 *	0.0000 *	0.0000	0.0000 *	0.0000 *
Master Comp Mass Frac (3-Mhexane)	0.0258 *	0.1577 *	0.0000	0.1577 *	0.0000 *
Master Comp Mass Frac (4-Mnonane)	0.0008 *	0.0118 *	0.0000	0.0118 *	0.0000 *

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NORWEGIAN UNIV OF
Burlington, MA
USA

Case Name: FERDIG2 RECYCLE.HSC

Unit Set: Oleekte

Date/Time: Tue Jun 12 09:00:31 2012

Workbook: Case (Main) (continued)

Compositions (continued)					Fluid Pkg:	All
Name	Fueloil/diesel/kerosene	HP steam in	Fueloil/diesel/kerosene	HP steam out		
Master Comp Mass Frac (Methane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (Ethane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (Propane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (i-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-Butane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (i-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-Pentane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-Hexane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-Heptane)	0.0006 *	0.0000 *	0.0006 *	0.0000		
Master Comp Mass Frac (n-Octane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-Nonane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-Decane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C11)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C12)	0.2488 *	0.0000 *	0.2488 *	0.0000		
Master Comp Mass Frac (n-C13)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C14)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C15)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C16)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C17)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C18)	0.1187 *	0.0000 *	0.1187 *	0.0000		
Master Comp Mass Frac (n-C19)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C20)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (n-C30)	0.0631 *	0.0000 *	0.0631 *	0.0000		
Master Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (H2O)	0.0000 *	1.0000 *	0.0000 *	1.0000		
Master Comp Mass Frac (Hydrogen)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (CO)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (CO2)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (3-Mhexane)	0.0000 *	0.0000 *	0.0000 *	0.0000		
Master Comp Mass Frac (4-Mnonane)	0.5687 *	0.0000 *	0.5687 *	0.0000		

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* Specified by user.

Appendix F – Electronic appendix

The files in this appendix are given electronically and the content is:

- HYSYS files for both cases (with/without LPG recycle)
- MATLAB codes
- Excel documents for three cases (without recycle, with recycle, with recycle and CO₂ emission cost)
- Earlier report

To run the MATLAB script it is important that the HYSYS file is already open