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Reducing the CO2 emissions of a gas cracker by reforming fuel gas

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Summary:

With the rising need for CO_2 reduction and the pressing two-degree target there is no doubt that measures must be made in the chemical process industry. Ethylene production by steam cracking is a mature and widespread technology. In addition, to being one of the most energy intensive processes, global emission from steam cracking exceeds 300 million tons of CO_2 every year.

This report presents the decarbonization options of the ethylene production, as well as production pathways from hydrocarbons to hydrogen. The main goal is to investigate if fuel replacement by reforming the current fuel to only hydrogen can cover the energy demand in a steam cracking furnace for ethylene production.

The selected method for hydrogen production is an autothermal reforming process (ATR) with integrated pre-combustion CO_2 capture. The process is simulated in Aspen HYSYS and partly maximized for the hydrogen production. The optimization is conducted as a result of examining five different configurations and nine case studies, including the most important input parameters.

The result was a system with a pressure of 2290kPa (in ATR), ST/C-ratio of 2, O2/C-ratio of 0.52, and an inlet temperature to the ATR of 750°C. The inlet temperature to the high and low-temperature water-gas-shift reactors was 300°C and 175°C, respectively. The inlet flow is 514.2kmole/h methane and 2976.3kmole/h hydrogen, where 95mol% of the hydrogen is separated prior to the reformation process. The simulation did not result in a system that can cover the energy demand by only reforming the current fuel to the cracking furnace. To cover the gap between the simulated and desired flow of hydrogen, an inlet flow of ethane was added to the process. By adding 22kmole/h of ethane, a sufficient amount of hydrogen flow was reached. Additionally, potential steam export was found to be 21.3MW, excluding the heat required for CO_2 and H2 separation unit(s).

Overall evaluation is that fuel replacement in industrial furnaces can have a significant impact towards decarbonization of energy intensive industries and that reforming traditional fuels containing hydrocarbons to hydrogen shows potential.

Preface

This project was written in the last semester of the master program "Process Technology" at the University of South Eastern Norway, as a part of the course FMH606. The aim was to investigate the option of reforming the fuel gas to a cracking furnace for reducing the related carbon emissions. Simulations were performed using Aspen HYSYS v12.

I deeply appreciate the time and guidance from my two supervisors Klaus-Joachim Jens and Lars Erik Øi throughout the semester. In addition, I would like to express my gratitude towards the people surrounding me in this period, for their support and patience.

Porsgrunn, 19th of May 2021

Emmy Kristine Lindeløff Rustad

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Nomenclature

ΔH_{int}	Enthalpy change
ΔT_{int}	Temperature interval
ACT	Accelerating CCS Technologies
APC	Advanced Process Control
AC	Alternating Current
ATR	Autothermal Reformer
BMTO	Biomass to olefins via methanol-to-olefins
CCS	Carbon Capture and Storage
CPO	Catalytic Partial Oxidation
CFTO	Coal to olefins via Fischer-Tropsch to olefins
CMTO	Coal to olefins via methanol-to-olefins pathway
CRE	Combined Reforming and Electrolysis
Comp	Compressor
CFD	Computational Fluid Dynamics
Co	Cooler
°C	Degree Celsius
Q	Energy [kW]
E	Exa (10^{18})
G	Giga (10^9)
g	Gram
GHG	Greenhouse Gas
HX	Heat Exchanger
HT	High Temperature
h	Hour
IGT	Industrial Green Tech
IEA	International Energy Agency
ISO	International Organization for Standardization

J	Joule
k	Kilo
kg	Kilogram
LCA	Life Cycle Assessment
LT	Low Temperature
$\dot{m}$	Mass flow [kg/h]
MER	Maximum Energy Recovery
MT	Medium Temperature
M	Mega (10^6)
MR	Membrane Reactor
MDEA	Methyl diethanolamine
mt	Metric ton
NOx	Nitrogen Oxides
Nm^3	Normal Cubic Meter
O2/C	Oxygen to Carbon ratio
Pa	Pascal
POX	Partial Oxidation (Non-catalytic)
PR	Peng Robinson
PSA	Pressure Swing Adsorption
PEM	Proton-Exchange Membrane
s	Second
Sep	Separator
SE-SMR	Sorption Enhanced Steam Methane Reforming
SE-WGS	Sorption Enhanced Water Gas Shift
Cp	Specific mass heat capacity [kJ/(kg*°C)]
Ts	Start Temperature [°C]
SMR	Steam Methane Reforming
ST/C	Steam to Carbon ratio

Tt	Target Temperature [°C]
T	Temperature [°C]
TLE	Transfer Line Exchange
VPSA	Vacuum Pressure Swing Adsorption
WGS	Water Gas Shift
W	Watt
wt%	Weight Percent

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1 Introduction

1.1 Motivation

Since the Second World War the importance of olefins has grown, along with the production and use of petrochemical products. Ethylene has a large repertoire of applications and is consumed at a remarkable high rate; therefore, it has a substantial effect on the global petrochemical industry [1].

With the Paris agreement from 2015, and the national goals of Norway towards a greener society, the exploration of different CO2 reduction methods has come to light. Industrial Green Tech (IGT) has a vision of making the industrial region in Grenland climate neutral by 2040 and have mapped out the current emission status and suggested some reduction possibilities. One of the methods that are suggested for evaluation is replacing the fuel to the crackers at INEOS, which currently consists of methane and hydrogen. If this fuel gas is reformed to pure hydrogen, it can potentially reduce the current emissions of CO2. [2]

1.2 Goals of the project

There are four overall goals of this project. The first goal is to make a literature study of the already available decarbonization options for a steam cracker. Hereunder falls the introduction to ethylene and a description of the traditional production method. The second goal is to investigate various pathways for producing hydrogen from hydrocarbon sources. The third goal is to select a suitable hydrogen production technique and simulate the process in Aspen HYSYS. The purpose of the simulation is to investegate if the system produces enough hydrogen from reformation of the fuel gas, so that is can replace the current heat supply to the furnace. Additionaly, different configurations and parameter varations should be conducted to maximize the production rate. The three stated goal lays the foundation to the fourth goal, which is evaluation of the suggested concept.

It should be clearified that this is a conceptual study and will therefore include a noteworthy amount of literature and theory prior to the simulation part. This is to provide a sufficient background knowlegde and to cover the requested preperation for a literature review, both for the cracking and reforming process. The task description is given in Appendix A.

1.3 Scope

It is not within the scope of this project to: 1) assess the economic aspects related to the simulated process, 2) create an optimized, ready-to-implement process solution, 3) technology selection for CO2 capture and H2 separation and purification or 4) propose the next steps for the captured CO2. Some aspects regarding CO2 capture and H2 separation will be presented, and it includes suggestions. With this borderline follows the lack of quantifying the energy consumption related to these process steps.

The reforming process is partly optimized for hydrogen production and the report includes suggestions for possible alterations and future work. However, it must be underlined that the

optimization of the suggested process are likely to have more potential and will probably require alterations once the economical ascpect is included.

1.4 Report structure

Chapter 2 presents a general introduction to ethylene and its industrial production. Fundamental information is provided, along with a brief process description of a typical ethylene production plant with a steam cracking furnace.

Chapter 3 presents different possibilities for decarbonizing ethylene production with focus on the steam cracking process.

Chapter 4 presents various concepts for producing hydrogen from hydrocarbon sources. Both mature and novel technologies are included.

Chapter 5 presents an introduction to the simulation tool Aspen HYSYS, a more detailed problem description, and a presentation of the base case.

Chapter 6 presents the simulations conducted in Aspen HYSYS with five different configurations (Case 0-5).

Chapter 7 presents an analysis of some of the simulations. First two burners with different fuel are compared, followed by investigating the effect of varying essential design parameters (case studies). Last in the chapter is a sixth simulation presented which is a system that is partly optimized for maximizing hydrogen production (Case 5).

Chapter 8 presents a pinch analysis of Case 5. The hot and cold utilities are calculated, and a potential steam export for the system is found. In addition is a suggested maximum energy recovery (MER) network presented.

Chapter 9 presents an evaluation and discussion of the covered topics and simulations.

Chapter 10 presents a conclusion.

2 A brief presentation of ethylene

This chapter introduces ethylene and its production by steam cracking. The first section is a general presentation. The second section describes the production steps and a steam cracking furnace. The third presents of the development and potential outlook.

2.1 Introducing ethylene

Ethylene is the most produced organic substance in the world and is a pillar in the chemical process industry. The ethylene molecule consists of two carbon and four hydrogen atoms and is an unsaturated hydrocarbon. It is not corrosive nor toxic, but flammable and colorless. Most of the ethylene is used to produce polyethylene (approximately 60%), polymers, and fibers. [1] Historically, naphta has been the favored feedstock option, followed by ethane in the regions which has natural gas more easily available. Ethane is the feedstock that provides the highest yields for ethylene, so at sites where ethylene is the primary product this might be more beneficial. In the twenty year period from 1995 to 2015, did the demand for ethylene doubled, mainly due to the increased use of plastic in the Middle East and China. [3]

2.2 Ethylene production

A scientist from Standard Oil got a patent in 1913 for the thermal cracking process. By the 1930s was the first commercial ethylene production plant built and started by Linde. The steam cracker was developed in the following decade and in the 1950s did ethylene become the primary input for synthesis.[4]

In 2000 the global capacity for production of all light olefins was about 150 million tons [5]. And to put the growth rate in perspective was ethylene alone consumed in a rate exceeding 150 million tons in 2017. Cracking of hydrocarbon is the dominating production pathway. The highly endothermic reaction requires high temperatures to produce the desired products. Combustion of fossil fuel to produce this heat adds to the emissions and energy demand, resulting in 1-2 tons of CO_2 for every ton of produced ethylene. The emission depends mainly on feedstock and the separation process. Steam cracking is a mature technology which has been optimized and developed for decades. Nevertheless, the steam cracking process alone used 3EJ by combustion of fossil fuels alone, making it the chemical industrial process with the highest energy demand. This resulted in an emission of 200 million tons of CO_2 in 2000 and 300 million tons CO_2 in 2019.[5, 6]

Cracking is the process where bonds between molecules are broken, more specifically the covalent bonds between the carbon atoms. This is a common way to refine hydrocarbons into new products. An example is making alkenes from alkanes. The cracking process depends highly on temperature and catalysts. The cracking technology can be divided into two major categories: Thermal and Fluid Catalytic cracking, where both has subcategories like steam cracking and hydrocracking, respectively. The different cracking methods operates under different conditions and has different products. What is valid for all is that every cracking process are highly energy intensive. [7]

2.2.1 Process description

Figure 2.1 illustrates a typical process block diagram over a cracking process for ethylene production. There are variations between production sites, dependent on feedstock and products. The steps are similar and it is only presented a general flow sheet with a light feedstock in this description. The feedstock is fed to the cracker which usually is a multi-tube furnace heated by combustion of fossil fuels. The feedstock is to a large extent decided by location and price. The cracking is done thermally with steam and is referred to as pyrolysis. [8]
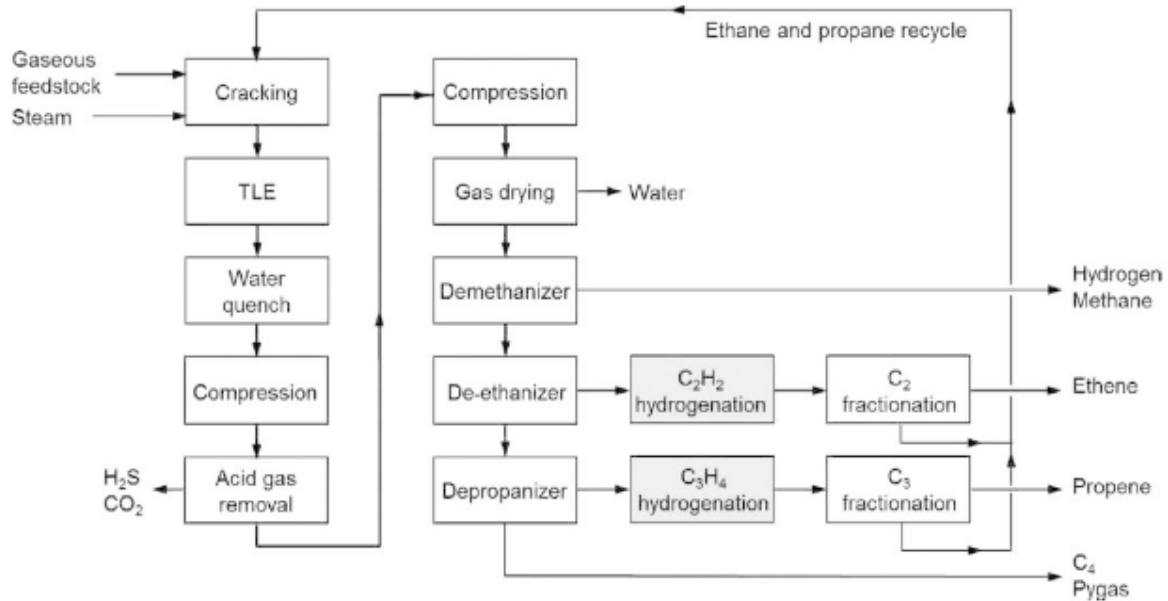
Figure 2.1 Block flow diagram over a typical ethylene production plant with gaseous feedstock (from [8])

Inside the cracking furnace numerous reactions are taking place and they can be divided into primary and secondary reactions. Primary reactions generally result in the desired product, and secondary reactions result in byproducts. The summary of this is presented in Table 2.1 and is based on a table from [9]. The overall goal is to maximize the primary reactions and to minimize the secondary reactions. The reactions are affected by inlet compostion, temperature, residence time, steam, partial pressure, reactor pressure, and quenching. Not suprisingly, a heavier feedstock is often related to larger amount of heavier products. It uses the steam as a heat carrier and diluent, which results in a high conversion. [8]

Table 2.1 Summary of primary and secondary reactions in a cracking furnace [9]

Primary reactions		Secondary reactions	
Feedstock and steam ➡	Ethylene	➡	C4 products
	Propylene		C5 products
	Acetylene		C6 products
	Hydrogen		C7 products
	Methane		Aromatics
	Etc.		Heavier products

After the cracking furnace the gas is sent to a transfer line exchange (TLE) and quenching prior to the compression in order to reduce secondary reactions. The next step might be removal of acid gas before a second compression step. The gas is often dried before the recovery section. The recovery (or fractionation) section separates the various components till a desired purity is reached. The fractionation section usually consists of distillation columns. Unreacted feedstock is traditionally resirculated to the furnace and gases.

2.2.2 Steam cracking furnace

A steam cracker with ethane as feedstock has an outlet stream consisting mainly of ethylene, unconverted ethane, hydrogen, methane and some amount ethyne, propane, propene, propadiene, butane butene, butadiene, pyrgas, and fuel oil [10]. INEOS has ethylene as their most important product and the separated methane and hydrogen is burned in the cracker as fuel. The outlet of the combusted fuel is primarily water and CO2, and is usually utilized for heating or steam export before being emitted to the atmosphere.

Figure 2.2 is an illustration of a steam cracking furnace (from [11]). It can be seen from the figure that the natural gas feedstock and steam is mixed prior to the cracker. The cracker is heated by fuel combustion together with air, this fuel can be a mix of methane and hydrogen from downstream separation. The exhaust gas from the fuel combustion is cooled down by steam prior to the outlet to the air. This direct emission point is normally what makes a steam cracking process highly carbon intensive. The feedstock which has been cracked exits the reactor and goes directly to be quenched. The quenching process is normally done by adding oil or steam.
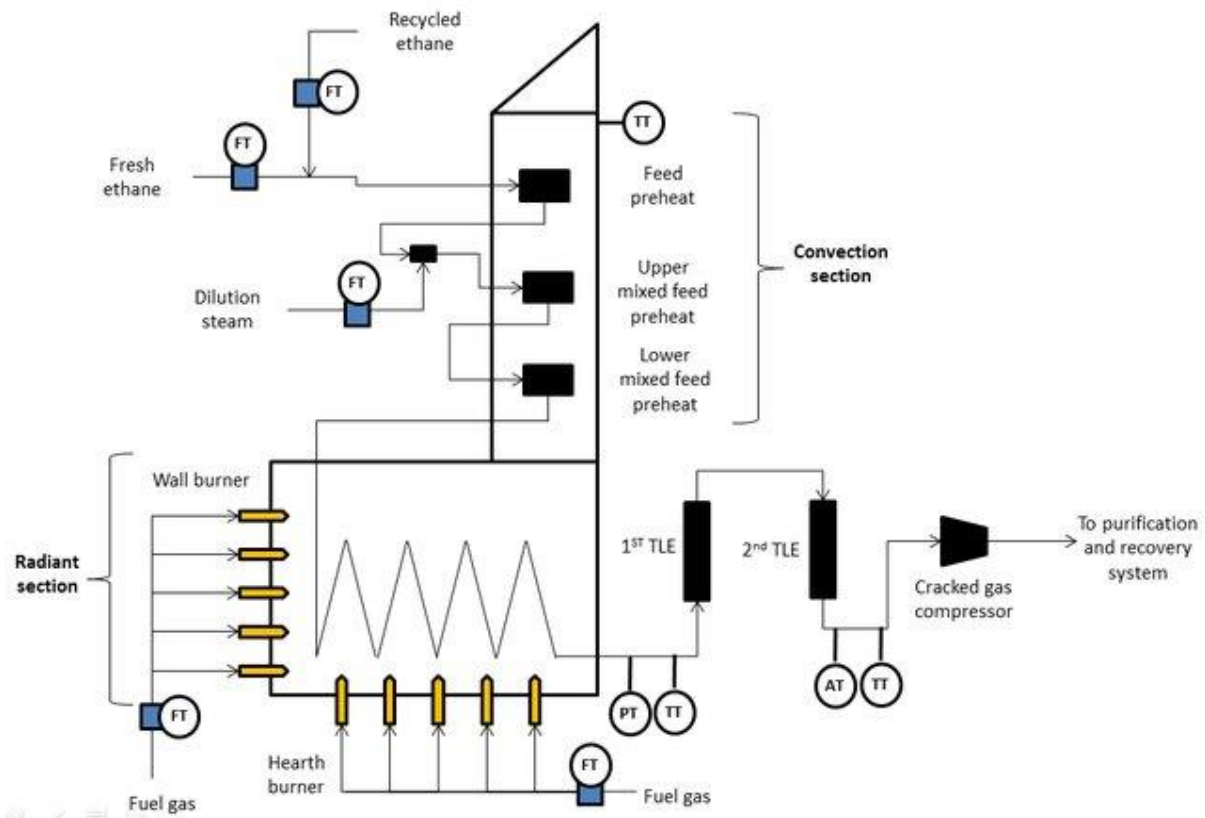
Figure 2.2 Illustration of a steam cracking furnace (from [11])

2.3 Development and outlook

Historically, the ethylene and economic growth rate has followed a similar trendline. This made it natural to assume that the COVID-19 pandemic that embossed most of 2020 would highly affect the ethylene production. Despite the effect of the pandemic the ethylene production continued to rise. The increased production is estimated to be approximately 1.5 million mt in 2020. The increase in 2021 is estimated to about 4 million mt and exceeding 6 million mt annually the following years. [12] In the upcoming years, the predicted increase in ethylene production is mainly caused by the demand for polyethylene. Other contributors are ethylene oxide and ethylene dichloride. A detailed and comprehensive study of the predicted market development can be found in literature [13-15].

The steam cracking method (as at INEOS) has a thermal efficiency over 90% which is remarkably high, making the improvement of the process challenging without drastic changes. However, when looking at work lost in the process (exergy) it is leading to the thought of intensifying the existing ethylene production is possible. [16] Other challenges regarding steam cracking are the undesired side reactions, catalyst deactivation and the very high energy requirement. All of this are potential areas for future development. [1]

Commercially, ethylene production by steam cracking has been done in fired heated tubular reactors. Nevertheless, the reasons to look for alternative methods are many; emissions, legislation, efficiency, cost, uncertainty in feedstock supply and independence from oil-based products, to mention some. One contribution to further development can be modelling of both

the cracker and the related systems. Modelling of the cracker has gotten a large amount of attention to strengthen the understanding of the involved reactions, optimal conditions, weak points, temperature, distribution, thermodynamics and etc. This can be done mathematically, empirically, by molecular kinetic models or mechanistic modelling. The available tools for simulating the process are many, but SPYRO model has been used to a large extent for cracking furnaces. When comparing experimental results from a cracker with SPYRO simulations it is within an acceptable range. [10] Other tools for simulating the process can be provided by, for example, Aspen HYSYS which will be used in project for simulating a reforming process. The possibility of more accurate simulation of industrial processes, such as cracking, has opened an enormous number of doors for rapid progress. This has highly impacted the swift changes in the chemical process industry over the last decades, and this rapid development can only be assumed to continue in the foreseeable future.

3 Decarbonizing the steam cracking process

This chapter provides an overview over various decarbonization options for a steam cracker and the ethylene production. The first section gives the reasoning and possible strategy for decarbonizing. The second section describes the decarbonization options related to feedstock, process intensification and optimization, followed by recycling and product solutions, and energy recovery. The third section presents the alternatives related to fuel substitution. The fourth section describes how carbon capture and storage (CCS) can be implemented. The fifth and last section offers an evaluation and selection of the described decarbonization ideas.

3.1 Reasoning and possible decarbonization strategy

The decarbonization of fuel for heat sources in the production of petrochemicals is essential. Currently, low carbon electricity can be available, but that is not the usual case for heat. Due to the enormous energy demand of petrochemical production, current fuel sources leads to high CO2 emissions. [3] Decarbonizing and/or reduction of the energy consumption in the industrial sector is therefore a necessity to reach the climate goals. The possibilities are many in the refinery sector and can be divided into seven categories, namely fuel substitution, feedstock substitution, process intensification and optimization, recycling, product solution, energy recovery and CCS or re-use [17]. Some options within these categories are yet to be competitive. The challenges often comes down to cost and availability of resources [3]. All the seven suggested methods will be briefly presented in the following subchapters. Since the scope of this report focuses on fuel substitution and carbon capture and storage, this will be the main focus area, and therefore these two are explained separately in section 3.3 and 3.4.

A reasonable starting point to systematically decarbonize a system is to develop a decarbonization strategy. In 2020 W. Falter et al [18] published an article with the title: "Decarbonization strategies in converging chemical and energy markets" where the strategy was to divide it into four overall steps. The first step revolves around the understanding and quantification of the current and future emission status, for all parts of the value chain. The second step is to identify and evaluate different decarbonization options and make these projects a priority. This evaluation includes both opportunities as well as technical and economic aspects. The focus for the third step is to identify possible challenges, future scenarios, and sensitivity of the decarbonization options. The fourth and final step is to make a goals and milestones for the decarbonization projects and complete the project and integrate the decarbonized system. The work presented in this project has focused on identification and evaluation, "step 2", but the whole strategy is important for the understanding of the bigger picture.

3.2 Presentation of selected decarbonization options

3.2.1 Feedstock substitution

The main feedstock for manufacturing ethylene is, as mentioned previously, ethane and naphtha. Both the process and the feedstock for a steam cracker have multiple replacement options. Ethylene can be derived from are biomass, coal, ethanol, syngas or via other sources such as methanol and chloromethane. [16]

To elaborate on one of the production steps towards producing ethylene from an alternative source, is methanol production briefly presented. The production method via methanol as an intermediate comes out far better in an environmental perspective than for example ethylene production from coal. The international energy agency greenhouse gas (IEAGHG) [3] considered and compared six routes for producing methanol, each from a different feedstock. A visual representation of the routes was summarized and graphically presented. This illustration is duplicated into this work and can be seen in Figure 3.1. The conclusion was that none of the routes were outstandingly superior, but biomass gasification and catalytic hydrogenation (with wind electrolysis) had the lowest global warming potential. The different
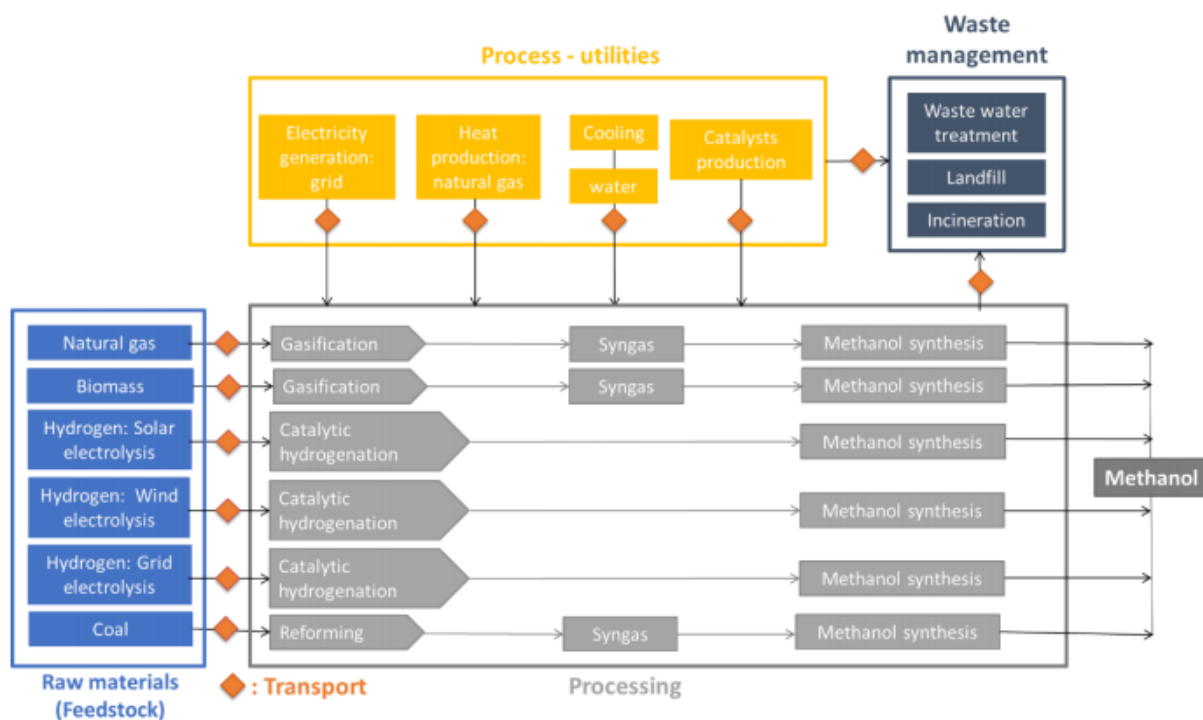
Figure 3.1 Visual presentation of six various pathways for methanol production (from [3])

Feedstock originating from biological sources may be the topic of greatest interest, due to the intensified interest it has received over the last years. A biological feedstock has its starting point from plants and the growing interest for this replacement is not without reason. Despite the fact that a naphtha steam cracker remains the most economical option, compared with bio-ethanol from sugar beets and bio-methanol from bio-waste, the reduced CO2 emission is making both solutions attractive. Especially if the pricing of CO2 is increased. However, the

crops must be produced without negatively affecting the food production. In order to realize more of these projects a cooperative effort from both industry and government must take place. [17]

Z. Zhao et al. [19] published in 2018 "Low-carbon roadmap of chemical production: A case study of ethylene in China". The study included a thorough LCA analysis of five alternative routes with ten different options to produce ethylene. Their findings were many and among them was the CO_2 emissions for the various pathways. There were also other production ways included in the assessment but three of them is illustrated below, including CO_2 emission with and without CCS. From top to bottom of Figure 3.2 is biomass to olefins via methanol-to-olefins (BMTO), coal to olefins via methanol-to-olefins pathway (CMTO), and coal to olefins via Fischer-Tropsch to olefins pathway (CFTO).
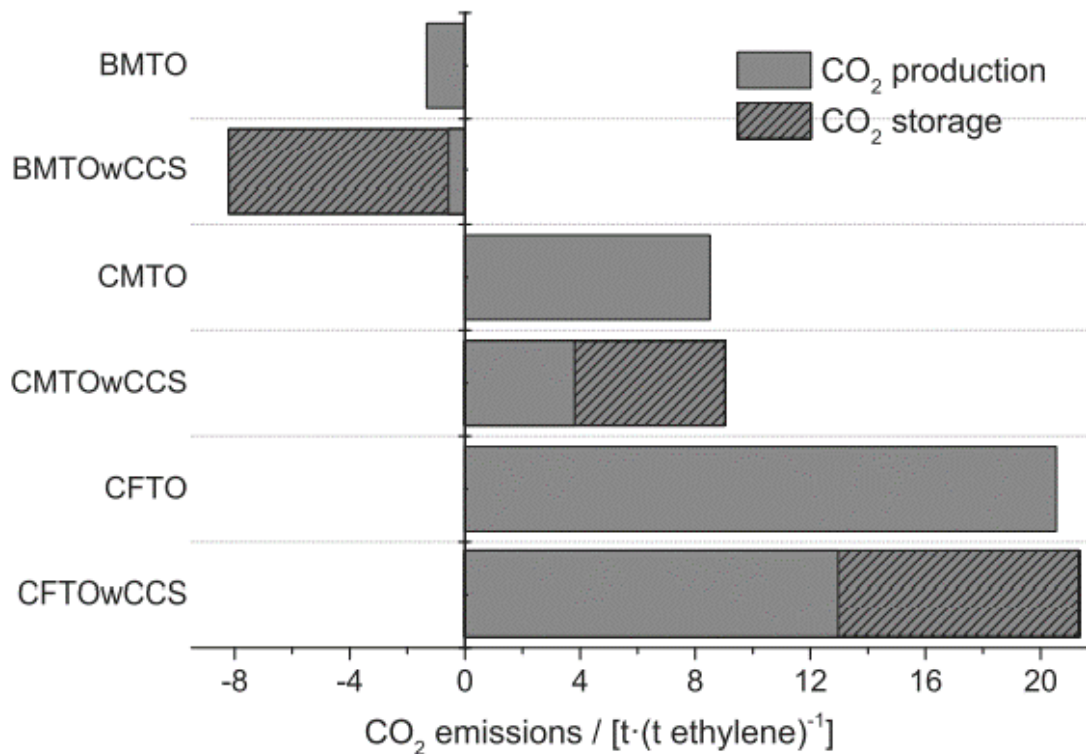
Figure 3.2 Comparison of the CO_2 emission through a life cycle for different production pathways (from [19])

The lowest emitting option was biomass to olefins via methanol-to-olefins (BMTO) with -1.3 ton CO_2 per ton ethylene. By implementing CO_2 capture it reduced to -8.2 ton CO_2 per ton ethylene. This illustrates the potential that lies in such substitution of the feedstock. [19]

3.2.2 Process intensification and optimization

It is difficult to predict which steps that are going to be the most influential for the future of chemical processes, but intensification undoubtedly plays an important role. Sine ethylene production is a highly energy intensive process, the input of energy must be done in an optimal way to ensure high energy utilization. To ensure this, the energy must be added in the right amount and location, at the right time and in the right form. Optimizing the energy need and

use (in for example a steam cracker or reformer) is therefore an important step towards decarbonization. [20]

Another important step towards decarbonization of ethylene production is to improve the already existing processes. Examples of how this can be done is increasing efficiency and heat recovery or reducing raw material consumption and energy demand. [17] Innovative technical solutions that are capable of producing the same amount in a more efficient and environmentally friendly way is of course desired. Advanced Process Control (APC) has proven to increase both efficiency and yields for the cracking furnace, increasing capacity and run time. The effect of APC on the cracking furnace performance has been notable. [21]

An important aspect for numerous chemical processes at an industrial scale, especially related to cracking and reforming processes, is catalyst utilization. Y. Gao et al [16] wrote "Recent Advances in Intensified Ethylene Production – A Review" in 2019. One of the most important part of that work was collecting and comparing the different reaction conditions, catalysts, and its performance. Underlining the importance and the gravity of impact a higher catalyst utilization would make, not only for the ethylene production, but for multiple other processes. The report also included a highly interesting comparison of alternative novel production methods for ethylene. Each of the presented technologies had both advantages and challenges and if interested, one can look it up there.

Last in this section a novel production method of ethylene from ethane will be introduced. It is included to make an example of how process innovation and intensification can contribute to the reduction of CO2. The system is an "Integrated Fluidized Bed Flameless Hydrogen Combustion (IFBHC)". The method claims a reduction in the CO2 emission by 80% and zero NOx emissions, in addition to higher yield of ethane and reduced investment and operational cost. The concept revovles around the use of an oxygen transport agent and a succsessful scale up was finished in june 2020. [22, 23]

3.2.3 Recycling and product solutions

There is more than one side of the aspect of recycling. One part is related to the recycling of used product, which in return gives lower raw material consumption. To exploit the potential that lies in the end-of-use of a product could affect the carbon footprint greatly, for example for plastic waste. A second part is recycling unconverted feedstock back into the process, again resulting in a lower raw material consumption. In the case of ethylene by cracking of ethane, could recirculation of unconverted ethane be an attractive option (if not done in the existing plant). A third part takes the recycling of internal process streams. [17]

By changing product solution, in this context, it is referred to three different scenarios. One is making the same products consist more of low-emitting components and less of high-emitting components. The second one is altering the product in such a way that the product requires less material and energy. The third one is changing the product such that the product is easier to recycle. [17]

The recycling and alterations of product solution is not a novel nor innovative idea in itself. But the quantity and quality of the recycled streams has a lot of potential and doors that has yet to be opened. There is an increasing interest to this part of intensification for reducing the carbon emission. To bring one of the many recent and relevant projects to light is a collaboration between SABIC, Renewi and Plastic Energy a fantastic example. The project

revolves around reducing the inflow naphtha to the steam cracker by replacing some of it with plastic waste that have been converted to feedstock. This reduces both the consumption of naphtha and the amount of plastic that are sent to incineration. The expected startup is in 2021. [17]

3.2.4 Energy recovery

It is no secret that poor utilization of high value streams with a high temperature is an potential energy sink at most ethylene production plants. The possible recovery is highly dependent on the existing plant. The highly energy intensive production makes the potential savings related to this likely to be notable. There are multiple aspects related to the energy recovery. In this sections some opportunities for energy savings related to ethylene production from natural gas systems by steam cracking mentioned. The following list includes some potential improvements to such systems can be. The list is based on a table from [24]:

- Increasing the efficincy of the turbines and compessors
- Improve the cracking process by reducing exergy losses
- Increase the efficiency in the steam system
- Reduce coke formation that leads to lower heat transfer
- Improve the burners and combustion section
- Optimize cracking conditions

The list above is related to reducing the energy use. The same work as that list is inspired from also stated a reduction possibility for the green house gas related to the ethylene production. The most important ones appears to be reduction of leakage, optimal cracking conditions, optimal heat transfer, reduction of equipment failure, and corrosion control. [24]

Exergy losses can be minimized by several means. For the cracking process it can for example be improved pre-heating of the flows to the cracker, have more but shorter tubes, reduce the pressure drop, and improved mixing. The compression and fractionation part is not covered extensively here, because the steam cracker itself is of most interest. However, it should be included that maximizing these efficiencies, for example by altering temperatures, pressures, and design, may prove to be beneficial if minimum carbon emissions are to be achieved. [25]

3.3 Fuel substitution

There are different fuels that can substitute the methane and hydrogen that currently are fed to the cracking furnace at INEOS. Due to the task description and the scope of the project is it here limited the two options; hydrogen and electricity. In addition is there a brief presentation of oxy-fuel combustion in this section, because even if it is not a fuel substitution in the common sense is it regarded here as a fuel enhancement and it therefore placed under this subsection.

3.3.1 Hydrogen

Substitution of the fuel used for heating the cracking furnace is, as stated in the previous sections, a highly attractive solution for reducing the carbon footprint. Assuming that the fuel

fed to the furnace today mainly conisists of hydrogen and methane that is a product of the cracking process, must the potential reduction be compared with this initial emission.

When hydrogen is combusted stoichiometrically with oxygen the product is water, as shown in equation (3.1). When a mix of hydrogen and methane are combusted, CO_2 is also found on the product side of the reaction. The energy release when hydrogen is combusted exceeds all other common fuels and has the highest energy per mass with 120.7kJ/g. Nevertheless, it is vital that the production of the hydrogen which are being combusted originates from a low-emission production in order to substantially reduce the CO_2 emission. In addition, comparing the combustion of hydrogen with methane only based on the energy per mass gives an inaccurate presentation of the energy available. Mainly due to the density. [26]

$$2H2 + O2 \rightarrow 2H2O \qquad\qquad (3.1)$$

The technical status related to using hydrogen as fuel to industrial furnaces is that burners with hydrogen as fuel is possible, but some challenges are encountered. The major one, compared with natural gas, is the potential increase in NOx emissions. Luckily, there has been breakthoughs in that area over the last years. Previously low NOx emissions for a hydrogen burner was only possible at specific, limited ranges of operating conditions. Now, there are avaible burner technologies with a more compact flame and advanced controlling, making the burner much more applicable for cracking furnaces. [27] CFD simulations on replacing the fuel to a fired heating furnace with hydrogen indicated no negative affect regarding operation of the heater. The fuel replacement was in the radiant section of the furnace. The NOx emission not drastically increased even if the temperature in the flame was high. The overall goal of the CFD simulation was to see how the flow, heat, and radiation was altered when using the same burner geometry but with different fuel. The result also showed that the distrubustion of heat changes with the fuel, where hydrogen was more uniform. The heat load was matching for both fuels and the the evaluation was that the performance was not lower with hydrogen as fuel. The applied geometry was rather simple and the work implies that the NOx emissions might change depending on burner design, firing rate, and the excess of air. To summarize was the results promising. [28]

Other challenges regarding the use and combustion of hydrogen is related to transportation and storage, as well as safety. However, producing and using the hydrogen on site makes some of these issures and concerns reduced or eliminated. If the hydrogen was to be transported, one could consider using an enery carrier such as ethanol. [26]

3.3.2 Oxy-fuel combustion

The concept of oxy-fuel combustion is simply to partially or fully replace the air used for combustion with oxygen and the technology can be retrofitted into existing systems. By removing the nitrogen from the inlet air is the NOx emission zero. Also, by replacing air with oxygen is the gas flow reduced, which leads to a lower heat loss and equipment size, as well as the characteristics in the combustion chamber is altered. In addition is CO_2 concentration in the outlet flue gas higher, making CCS more favorable. The burning of fuel with pure oxygen

increases the temperature and a recirculating stream is needed to compensate for this. The oxygen production unit is usually a cost and energy intensive device. [29]

There has been developed extensive models and computational fluid dynamics (CFD) simulations over burners and combustion of fuels with increased oxygen flow [30, 31]. For a steam methane reforming (SMR) furnace, which in many ways resembles a cracking furnace, was the consequence of oxygen enrichment lower NOx emissions, higher CO_2 concentration in the flue gas and improved heat transfer in the furnace, as predicted. These phenomena can be explained by the increased flame temperature and the reduction in heat lost via the nitrogen through the exhaust gas from the furnace. An advantage of implementing oxy-fuel combustion at already existing plants is that the implementation is quite easy, meaning that the alterations to the existing process and equipment are minor. [32]

3.3.3 Electricity

Decarbonizing of and by electricity is generally an important part of most industrial plans that focus on lowering the carbon emission. Multiple decarbonization roadmaps for energy intensive chemical process industry and electricity is available in literature [33-35]

Approximately 70% of the emissions from the refinery sector comes from thermal processes, dominated by gas-fired furnaces and steam generation. Decarbonizing this by electrifying these process operations would have a massive impact. The electrification possibility is highly dependent on availability of low-emission electrical sources, as well as the electricity price. [36]

Electric heaters have several advantages compared with furnaces that receive energy via burners, some of which will be pointed out. Firstly, one can obtain a higher heat release in a smaller volume making the size of the equipment/furnaces lower. Secondly, the heat is distributed more uniformly leading to advantages related to products stabilization and catalyst utilization. Thirdly, easier, and more consistent control of the temperature. Fourthly, the start-up time is likely to be lowered. [37]

A breakthrough in the ethylene and olefins production is the design and implementation of the first electric steam cracker. This is currently being planned and projected by BASF, SABIC and Linde. The news was published in late in March 2021 and the electric cracking furnace has a planned start-up in two years from now, in 2023, and with up to 90% CO_2 reduction. [38]

3.4 Carbon capture and storage

Carbon capture and storage (CCS) will inevitably continue to grow and be a part in any CO_2 reduction plan for today and for the near future. The industrial sector has already implemented a variety of technical solutions to capture, transport, store and/or utilize the CO_2 that previously was emitted to the atmosphere. However, all the challenges related to technology, cost, energy requirement, and energy efficiency is yet to be overcome. In order to implement a viable technology for CO_2 reduction and/or capture in the industries with a notable reduction potential must it be reasonable economically, environmentally, practically, and socially. CCS at an ethylene production plant could be just that.

Some sections of the report (4.2.2) include more on CO_2 capture and some of the advantages that follows with it. In this section will the CO_2 capture units that can be implemented in a

hydrocarbon steam cracker plant be briefly described. Covering this part of the CO2 reduction in detail is note regarded as necessary since available technologies for CO2 capture and CO2 separation techniques are many and are covered extensively in literature [39-41]. It goes without saying that capturing the CO2 pre- or post-combustion will reduce the carbon emissions.

The dominating and mature technology is absorption with its high efficiency of over 90%. The downside is that is has a high demand of energy related to the regeneration of the absorbent. Adsorption can have efficiencies exceeding 85% and the absorbent is recyclable. The desorption process is energy intensive and require high temperatures. Membrane separation have yet to develop a feasible and affordable solution to the related operational problems, for example fouling, but the method can separate over 80% of the CO2 and the technology is highly developed for other substances. Another separation method which has received more attention over the last years and can be applied for CO2 recovery is cryogenic distillation. The downside of this technology is that the energy requirement is high and the CO2 fraction in the inlet most be more then 0.9wt%. Some less mature technologies that still need more development and research or experience on an industrial scale is chemical looping combustion and hydrate based separation. [41] A couple of other possibilities for capturing the CO2 related to the reforming (and not cracking) process will be mentioned in chapter 4.

3.5 Evaluation and selection of decarbonization options

An overview over the most probable decarbonization options for a steam cracker and the ethylene production has been given. The focus has been mostly directed towards the production itself, and not included measures that can be made by the consumer. There are other alternatives besides the ones presented here but the presentation is adequate to its purpose, namely providing an overview and underline that; Yes, there are several possibilities for reducing the carbon emission related to ethylene production by steam cracking. Evaluating and selecting the best suitable decarbonization is challenging when the specific to the plant site (for example INEOS) are not available and/or publishable, and the targets might vary between the different production sites.

The work plan given in the task description states that a literature evaluation for reducing the CO2 emissions should be prepared. Even if no specific conclusion is made from the literature evaluation, some lines can be drawn from the information. It appears that process intensification and maximizing the efficiencies play a central role if current plant layouts are to be kept. Especially for the cracking furnace. This can be achieved by optimizing the cracking condition and heat transfer. In addition, improving and maximizing the recycling of process flows and energy streams might benefit in reducing the carbon emission. When it comes to feedstock substitution appears biological sources promising. Regarding fuel substitution is all three presented options (hydrogen, electricity, and oxy-fuel combustion) likely to be implemented as an alternative to the current fuel. The findings are not revolutionary or surprising but is merely meant as an overview to where one could start the process of decarbonizing a steam cracking process for ethylene production.

However, as clearly stated in the task description reforming of fuel gas to pure hydrogen as the decarbonization option will be further evaluated. As the literature study showed, reforming fuel source to pure hydrogen is a viable option for decarbonization, justifying further investigation.

4 Reforming concepts and hydrogen production technologies

This chapter presents the reforming concepts for producing hydrogen originating from hydrocarbon sources. The first section introduces hydrogen and its production. The second section presents mature and well-tested reforming technologies. The third section presents some novel and/or alternative production. Lastly, in the fourth section is the reasoning behind the technology selection.

4.1 Introducing hydrogen and its production

As stated previously is replacing the fuel used as heat supply the cracking furnace with hydrogen the topic for further discussion in this report. Even if there are other methods to produce hydrogen available, the production methods which has methane or other light hydrocarbons as primary input are the ones that will be presented in this chapter. Producing hydrogen from natural gas sources such as methane makes up around 90% of the global hydrogen production. It can be produced multiple ways, but currently SMR is the leading technology. The SMR has a carbon footprint of approximatly 0.81kg of CO_2/Nm^3 H2 produced (modern plant) [42]. Approximately 40% of this CO2 is from the combustion of fuel in the furnaces and the remaining 60% is from the feedstock to the steam reforming process. However, a viable and attractive option to make this process a low-carbon producing method is to combine the reforming process with CCS. Hydrogen produced in such manners is referred to as blue hydrogen. In order to be categorized as green hydrogen most the feedstock originate from a renewable source, for example water that undergoes elctrolysis with electricity from a renewable source, to produce hydrogen and oxygen. If hydrogen is produced with by SMR combined with CCS will it never reach the green hydrogen mark, due to the fact that the CO2 capture rate is below 100% (typically range from 50-90%). [43]

Hydrogen as fuel substitution was briefly presented in section 3.3.1. In this section the focus will be on the production of the hydrogen that can substitute the methane to the furnace. The main difference between producing hydrogen for combustion purposes compared to other applications is that the purity requirement of the hydrogen is generally lower. The hydrogen content and other purity requirements are highly depended on the area of use. A commoner for downstream processes is limitations due to catalyst degradation and contamination. The contaminations are usually sulfur, CO, CO2, and H2O but can be other trace substances as well (for example N2, Na, He, K, and Ar). For refining the lower limit is around 0.95mol%, for ammonia production around 24 mol% (N2 is the main component) and for gas turbines the purity can be quite low. Other applications like PEM fuel cells can be in the range of 0.50 to 0.9997mol% where the upper section refer to hydrogen for automobiles. When it comes to power and heating purposes in industry the ISO standard is at 0.999mol% but this limit is occasionally not regarded as an absolute. It should be evaluated for each specific case and this lower limit is likely to decrease in the near future. [44]

Hydrogen production from hydrocarbon sources is most commonly dived into 3 sections. First a section to produce syngas, short for synthesis gas, which in this context refers to a mixture of H2 and CO. The syngas can originate from both natural gas, heavier hydrocarbons, or

pulverized coal. Depending on application and the following process is the syngas sent for processing in a second section. This processing can be water-gas-shift (WGS) reaction, CO removal, or other treatments to obtain the desired composition and/or ratios. The third section relates to reaching the specifications of the H2, in regards to purity and content of different contaminations. [8]

4.2 Mature methods for hydrogen production originating from hydrocarbons

Reforming, in this context, refers to the process in which hydrocarbons are altered to create new substances with higher value or with more desired properties [45]. Reforming of natural gas to hydrogen is by far the most widespread technology. Therefore, this will be presented more thoroughly in the upcoming section. Not all reforming methods will be presented, only the ones regarded as the most probable for implementation at a plant such as INEOS. If interested one can find information about other methods (such as plasma, aqueous phase reforming, dry reforming) in literature [46, 47].

4.2.1 Steam Methane Reforming (SMR)

Steam reforming of natural gas over a catalyst has a long history and is the most common and widespread method to produce hydrogen in an industrial scale (48% of the worlds production). The hydrocarbons split with help of steam and high temperatures, making it possible for the hydrogen atoms to form the desired hydrogen molecule. The product after the reformer is mainly H2, CO2, CO and H2O, and the set of reactions is globally endothermic. The dominating reactions involved in the process presented in equation (4.1) to (4.3) (negative sign indicating exothermic reaction and positive sign indicating endothermic reaction). [26]

$$\Delta H \ [\frac{kJ}{mole}]$$

$$CH4 + H2O \rightarrow CO + 3H2 \qquad +206 \qquad (4.1)$$

$$CO + H2O \rightarrow CO2 + H2 \qquad -41 \qquad (4.2)$$

$$CH4 + CO2 \rightarrow 2CO + 2H2 \qquad +247 \qquad (4.3)$$
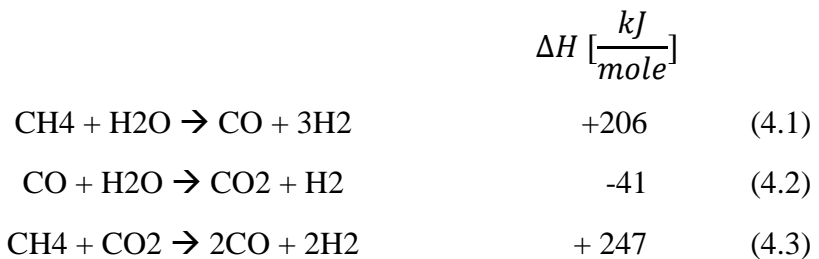
Figure 4.1 shows a flow diagram over a traditional steam reformer process. The gas input is removed of sulfur, to avoid catalyst deactivation, before it enters the reformer along with the steam. The conversion and the produced products are influenced by the feedstock, steam-to-carbon ratio, temperature, pressure, catalyst, and the residence time. The output of the reformer goes into the WGS section, which is most commonly is done in two steps, high- and low temperature. The goal of this step is to lower the CO content and raise the H2 content. Last step is a purification unit (for example pressure swing adsorption (PSA)) where the hydrogen can reach a purity of 99.99vol%. All other gases then hydrogen is traditionally absorbed (for example on activated carbon). [26]
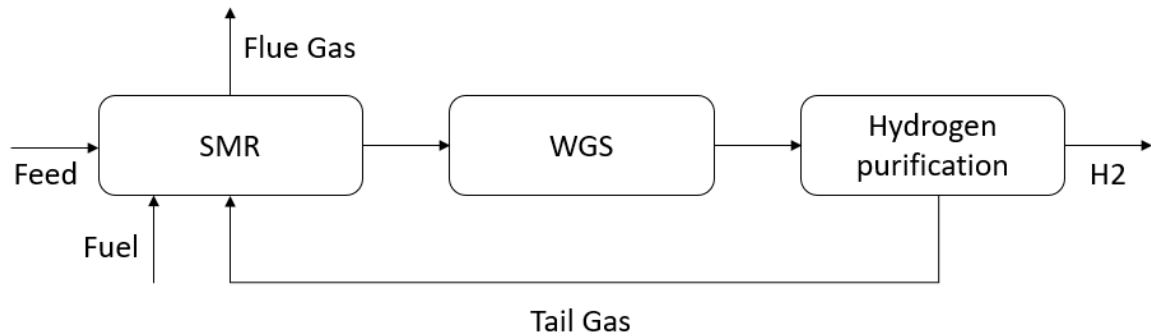
Figure 4.1 Flow diagram over a traditional SMR process

4.2.2 Steam Methane Reforming with CO2 capture (SMR+)

SMR+ in this report refers to the standard SMR with integrated CO2 capture. IEAGHG published in 2017 "Techno-Economic Evaluation of SMR Based Standalone (Merchant) Hydrogen Plant with CCS" [42] with a number of highly interesting findings. It was investigating numerous energy intensive industries and the findings included that further reduction of CO2 emissions from an SMR plant could only be done by integrating CCS, for modern hydrogen plants. This is since modern SMR pant operates at efficiencies close to the theoretical minimum (10% and above). Despite this is there only three SMR plants in operation which has an integrated CCS, located in USA, Canada, and Japan. The CCS was evaluated at three different locations in this, as illustrated in Figure 4.2. All cases were evaluated both by efficiency and cost and was compared to the base case in the study, which had natural gas as fuel for most cases. One exception was to recycle of a tail gas to the burners, enriching it with hydrogen. Which is conceptually similar to the idea presented in this work. The case presented had an increased CO2 avoidance cost and needed upscale to produce a reach the production goal which again led to an increased natural gas consumption.
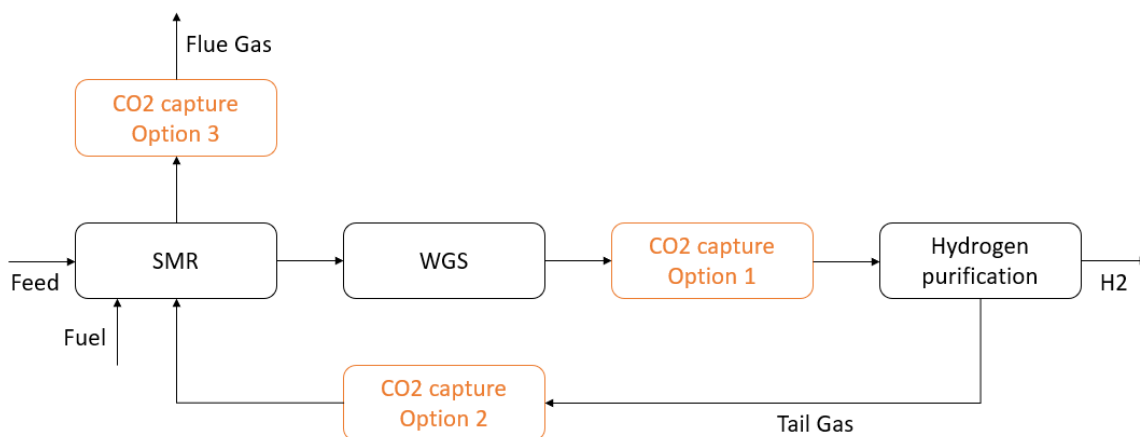
Figure 4.2 Flow chart over possible CO2 capture locations in a SMR system

CO2 capture associated with steam methane reforming can be divided into three categories, namely pre-, post-, and oxyfuel-combustion. Post-combustion has the disadvantage of low partial pressure and concentration of CO2, in addition to the usually large volumetric flows. This usually results in a high energy demand and the need of equipment with high capacity. Oxy-fuel combustion replaces the air with pure oxygen but is rarely economical due to the high investment and operational cost related to the production of the oxygen (as explained in section 3.3.2). Lastly, pre-combustion is also costly but shows an enormous potential. [8] As can be seen from Figure 4.2 are there two alternatives from capturing CO2 prior to the combustion, namely option 1 and 2. When comparing the three CO2 capture options the capture rate of option 3 is highest with 90%, followed by option 1 at 56% and option 2 at 54%. From an economical viewpoint it has been found that increasing capture rate causes an increase in the levelized cost of H2 and the CO2 avoidance cost higher. [43] This calculation and comparison does not take into account the possibility to include a hydrogen purification step for further utilization for the pre-combustion options. Taking this into consideration could affect some of the numbers, but the trendline is unlikely to be extremely altered. The ELEGANCY project, which is a part is the ACT (Accelerating CCS Technologies), developed a state-of-the-art flow sheet over a SMR system in order to produce hydrogen with low carbon emission from hydrocarbons. This was based on the study mentioned initially and if interested one can find it there. [42, 43]

If the CO2 are to be captured after the WGS (shifted syngas) is activated methyl-diethanolamine (MDEA) in a chemical absorption process regarded as the current state-of-the-art technology. The inlet natural gas increased with $0.46MJ/Nm^3$ H2 and reduced the CO2 by 54% when this technology was tested, compared to the base case in the research (The base gas had an inlet flow of $14.21MJ/Nm^3$). The CO2 was captured from the syngas after the shift reactors (option 1). When placing the CO2 capture location to option 2 was did the natural gas input increase with $0.59MJ/Nm^3$ H2 and the CO2 reduction was 52%. For the H2 purification step is PSA considered as the state-of-the-art. [42]

Alternative options are a combination of some of the process steps. For example, the WGS and CO2 capture in the single process operation called sorption enhanced water gas shift (SEWGS), which is explained further in section 4.3.3. [48, 49]

4.2.3 Partial oxidation (POX) and catalytic partial oxidation (CPO)

Partial oxidation is a manufacturing route where the required thermal energy is supplied internally. In contrast to a fired heated reactor (such as SMR) where the heat is supplied externally by combusting fuel (for example methane). The internal combustion is obtained by adding oxygen which oxidize the inlet stream of hydrocarbons. This results in reactions which in total are highly exothermic. The reactions are not reversible in the process conditions of interest, eliminating the dependence of external energy supply. This method makes use of the produced water instead of letting it exit as exhaust. There are two variations of partial oxidation which will be described in this section, namely non-catalytic partial oxidation (POX) and catalytic partial oxidation (CPO). A third method will be described separately in the next section, namely the autothermal reforming (ATR). [50]

The POX does not utilize a catalyst, making the technology dependent on high temperature if high conversions of methane are to be reached. In addition, the high temperature will reduce some of the soot formation. However, this production method is more often than not

implemented together with a soot reduction unit. A normal way to cope with soot formation is to add a specific amount of steam but in a POX system, the steam will cause a lowered temperature, which again increases the soot formation, making this coping method unfavorable. The CPO separates from the POX by having a catalytic reactor, making the required temperature lower for the same conversion. The type of catalyst that are utilized varies but an example is rhodium monolith, and the subject is under constant research and development. Both the CPO and the POX separates from the ATR by the lack of a burner. [50]

4.2.4 Autothermal reforming (ATR)

Autothermal reforming is a highly developed and well-tested technology and was first developed by SBA and BASF already in the 1930s. It is a combination of SMR and POX, where the reactor consists of a burner, a combustion section, and a catalyst bed section. This is illustrated in Figure 4.3. The methane is fed into the top section along with steam and oxygen. Firstly, following the exothermic reaction (4.4). The surplus heat is utilized in the endothermic section in the catalytic bed, where the two reactions (4.5) and (4.6) occurs. This combination of reactions is making the reactor self-supplied with energy. [50]

$$\Delta H \left[\frac{kJ}{mole} \right]$$

$$CH4 + 1.5O2 \rightarrow CO + 2H2O \qquad +519 \qquad (4.4)$$

$$CH4 + H2O \rightarrow CO + 3H2 \qquad -206 \qquad (4.5)$$

$$CO + H2O \rightarrow CO2 + H2 \qquad +41 \qquad (4.6)$$
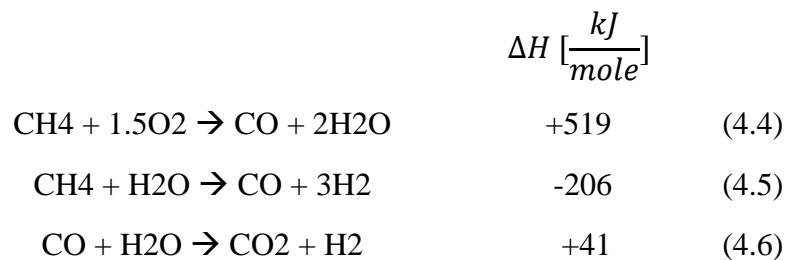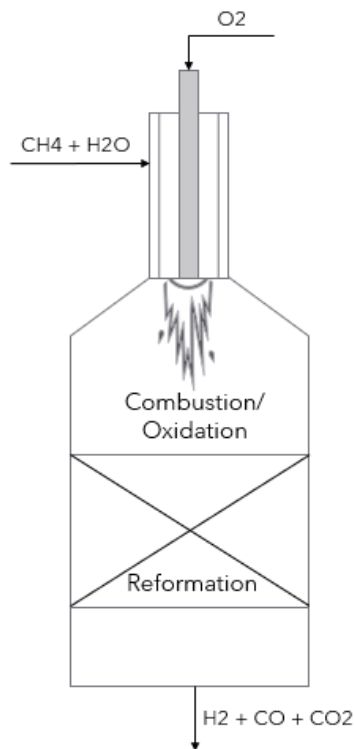
Figure 4.3 Illustration of an ATR (based on a figure from [50])

Compared to a fired furnace (SMR) the ATR is a system with reduced size and complexity. With no external heat supply required, the fuel cost to the reformer will disappear and lead to a reduction in the CO2 emission. Another advantage is that the ATR needs less water than a SMR. This is because the high temperature in an ATR leads to a high methane conversion without the water. Additionally, oxygen helps with the prohibition of soot formation. A disadvantage is that the oxygen production and consumption is expensive. [51] There is a balance between the inlet oxygen flow rate and the temperature in the ATR, where more oxygen will lead to higher temperature. However, the temperature is limited by the material and the constructional cost. The combination of a SMR and ATR is in some cases beneficial and are referred to as a combined reformer system. Studies have indicated that such a system can increase the production of syngas by 25.3% and reduce the oxygen consumption. Such a system will not be described further here. [52]

4.3 Advanced, novel and/or promising methods for hydrogen production originating from hydrocarbons

Apart from the aforementioned technologies for reformation of natural gas to form hydrogen there are a couple of other possibilities that will be briefly presented. Most of these technologies is not yet commercially available for large-scale production sites but shows potential and can therefore be highly interesting for the future. Some of the methods presented in the following sections was presented with purity, efficiency, temperature ranges and challenges in the report by M. Voldsund et. al [44]. It is inspired and referred to this work on several occasions and it is encouraged to look to this for more details and process specifics.

4.3.1 Methane pyrolysis

Methane pyrolysis is a technology where methane is thermally broken down to its fundamental elements carbon and hydrogen and has been studied for over a century. What separates this technology from the other processes is that the outlet gas does not include any CO2. Instead, the carbon is taken out as a solid and the outlet gas does not need a downstream purification or separation step. A clear upside of this technology is if the hydrogen produced by this method replaces hydrogen produced from higher-emitting sources, the CO2 reduction will be thereafter. Compared to other CO2-free methods for hydrogen production, for example water electrolysis with a renewable energy source, is methane pyrolysis favorable from an energetically viewpoint. The downside of this technology is that there is currently not a big market for the solid carbon, but of course this may change over time. And even if the energy efficiency of a methane pyrolysis process is competitive with SMR with CCS (58% compared to 60%), is the challenges related to the deactivation of the solid catalyst in the methane pyrolysis not at a satisfactory level. The catalyst will reduce the reaction temperature but the possibilities for development are numerous. [53]

4.3.2 Integrated membrane reactors

Membrane reactors for the purpose of reforming methane into syngas can be a highly attractive solution. Membrane reactors has since 1996 only grown and especially around those who are CO2 or H2 selective, were the latter affect the conversion most [44]. The properties of a membrane and the selection of the parameters is highly dependent on the area of use. In this context it refers to the choice between a membrane with selectivity towards hydrogen or a selectivity towards CO2. If the CO2 are to be transported the purity requirements are high, and the same goes for hydrogen. For the purpose of concept explanation let us assume that a relatively pure hydrogen stream is desirable. An example that has been under development is than to use a palladium membrane with a selectivity that is high for hydrogen. This membrane is placed together with a catalyst bed, making the conversion higher since the equilibrium is constantly moved when hydrogen is extracted. This setup has both been simulated and experimented on, achieving a temperature decrease (to approximately 700℃) without reducing the conversion of methane. [50]

The requirements for the membrane are not few. Both since the reforming takes place between 500 and 900℃ and because the high pressure and durability it needs. Also, to be competitive the transport of hydrogen through the membrane must be in the same range as the reaction and the membrane needs to have some tolerance for contaminations. It should also be mentioned that a membrane reactor system is also an option for the WGS reactor that usually is placed downstream of a reforming process, but the technology is currently transitioning from lab to pilot scale. The SMR, WGS and hydrogen purification can be combined in a SMR-MR (Steam Methane Reforming Membrane Reactor). The system can be illustrated as in Figure 4.4 and the system is referred to as integrated since there (potentially) is no need to further purify the CO2 with the exception of water removal. This again depends on application.
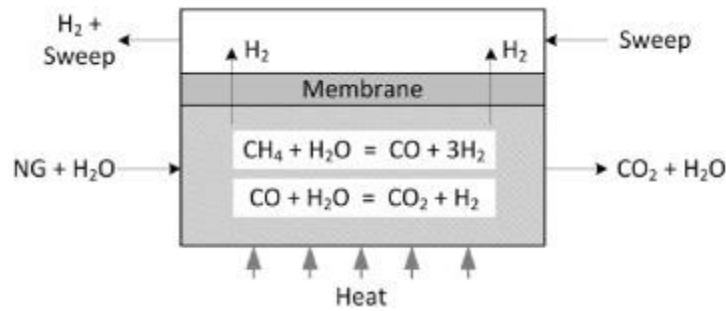
Figure 4.4 Illustration of a SMR-MR (from [44])

There is a thermal energy requirement to this system and conversion is higher at elevated temperatures and can be furthered boosted be adding a sweep. Alternatively, can membrane reactor systems that operate favorable at variating conditions be operated sequentially. A project by Tokyo Gas has tested such a system for over 3000 hours and the purity of the hydrogen was close to 100%. The efficiency was exceeding 70% but there is doubt of the cost, ability to last over time and temperature control, resulting in a need for more testing prior to a possible commercialization. A couple other novel membrane reactor configurations is micro membrane reactors and fluidized bed membrane reactors, but these will not be described in this report. [44]

4.3.3 Integrated sorption-enhanced systems

When utilizing absorbents to remove one of the components on the product side of the reaction (4.1) or (4.2), for example CO2, is the equilibrium continuously moved. Since the reaction is equilibrium limited prior to the removal of CO2 will the hydrogen production increase when CO2 is absorbed by an absorbent. This concept has acceptable conversions of the methane to produce hydrogen even at lowered temperatures. There are challenges regarding an absorbent which is affordable to purchase and regenerate, and simultaneously is stable with a satisfactory level of adsorption capacity and fast enough reaction kinetics. Nevertheless, there are alternatives that may meet the high requirements, one example is calcium oxide with addition of NaOH. This concept can be taken into practice in two purposes which are relevant in this project. First is the Sorption Enhanced Steam Methane Reforming (SE-SMR) and second is the Sorption Enhanced Water Gas Shift (SE-WGS). The principle is the same even is the desired input and output is different. The concept can be both be continuous or semi-continuous. Continuous with a circulating fluidized bed reactor, one for main reaction and one for sorbent regeneration (which appears as the better solution for the SE-SMR). Semi-continuous with multiple reactors where the different reactors are at a different step. The concept with the SE-WGS went from lab to pilot scale as a part of the Horizon 2020 which began in 2015. [44]

The SE-SMR operates at elevated temperatures compared to the SE-WGS and it includes both the reforming reactions and the WGS reactions. Even so, the temperatures in a SE-SMR are lower (can be around 600°C) than for a traditional SMR (can be around 1000°C). The road towards commercialization is a little longer than for the SE-WGS but has undergone lab-scale testing. ZEG Power had utilized the concept and are investigating the performance when producing electric power together with hydrogen in a fuel cell. [44]

There are two major advantages to implement a SE-WGS system compared to the traditional setup with two WGS in series. A SE-WGS utilizes a catalyst designed for WGS reaction and

an absorbent for the CO2 capture that function probably even at elevated temperatures. Leading to a system that has a cooling and heating requirement that is lower compared to systems which cool the gas before the WGS and reheats it before the CO2 capture unit. The other advantage is that the number of process units are lowered. [35]

4.3.4 Chemical looping variations

Looping of chemicals is neither new nor innovative in the chemical process industry. Even if there are several variations of this that can be relevant, only one will be described in this section. Other configurations and variations can be found in the literature. Chemical looping can be of oxygen which can be used in technologies like POX, CPO and ATR which all has oxygen as an input stream. The chemical looping process which is emphasized in this section is for the syngas, as described by M. Voldsund et al. [44]. The suggested setup consists of three reactors, namely fuel-, steam-, and air-reactor. The syngas is fed into a fuel reactor along with an oxygen carrier and the product is CO2, H2O, and the reduced carrier. The next step is the steam reactor where the water partly oxidized the carrier and produces more H2. The third step is an air reactor where the carrier is met with oxygen to be fully oxidized. The carrier is this way looped in circles between the three reactors. This method has the potential to produce both H2 and CO2 with high purity, separating is from the other method presented. The challenges related to this technology related to the oxygen carriers, more specifically finding carries that are stable after more than a few rounds in the system. [44]

4.3.5 Electric reforming

As previously mentioned, electrification of furnaces can greatly reduce the carbon footprint, if the electricity comes for a renewable energy source. This electrification of industrial furnaces and boilers is now included in multiple roadmaps towards a greener industrial sector [17, 36, 54]. S.T. Wissmann et al. [55] conducted lab-scaled experiments and the results were highly promising. The estimated CO2 and equipment size reduction was remarkable, in addition to the higher catalyst utilization and heat flux advantages. To illustrate the potential reduction in reformer size versus the methane conversion it is included a visual presentation that was made by the aforementioned authors, see Figure 4.5.
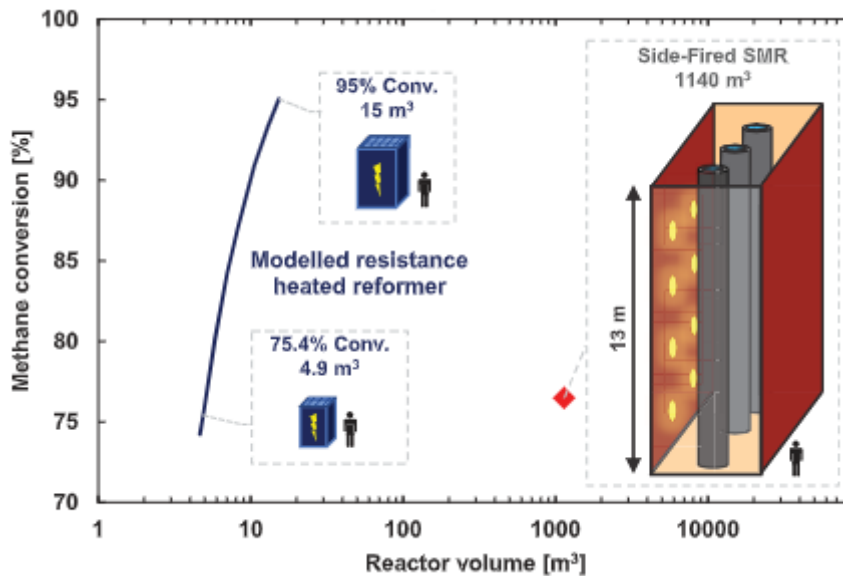
Figure 4.5 Visual presentation of a traditional SMR compared to an electric reformer (from [55])

Energy in the form of electricity or electromagnetic fields can be added to the furnace and/or boilers in a few different ways. Which technology that are utilized depends mainly on application, temperature, and material. All technology types fall under the two overall categories, direct and indirect heating. Direct heating has a flowing current through a direct connection with no intermediate medium or material. Direct heating is more suitable at lower temperatures and offers higher efficiency. Indirect heating is when firstly a medium is heated, then secondly the heated medium is heating another medium. This way of heating has a lower efficiency but is more suitable for higher temperature and pressure. [56]

Within the direct and indirect electric heating, there are multiple possible technology options. An overview of the different technologies for electric heated furnaces can be found in a report by V.P. Semeijn and K.M. Schure [57]. The five subcategories presented in the report were Resistance-, Arc-, Infrared-, Dielectric- and Induction-heating. Each with a temperature range and the most common industrial area for implementation. S.T. Wissmann et al. [55] experiments used direct resistive heating meaning that the energy supplied is used directly. This was done by attaching an AC current along the wall of the reactor, which had copper sockets at the outer surface. This system eliminates the gas heated section and enhances the thermal efficiency, resulting in a system with a great competitive advantage.

To summarize can it be said that electrified methane reforming definitely is an area of great interest and potential, but there is still a way to go before they can be commercially available. Because even if the use of electricity for heating is a traditional and familiar technology is the implementation of this to a refinery yet to be done. The upscaling to large-scale production from lab-scale usually come with high uncertainty and both known and unknown challenges. To minimize these risks should more testing, simulation and analysis be completed. [36]

4.4 Technology selection

When considering the systems described above it must be clarified that this evaluation is not detailed. This section is meant as an explanation for the choices and thoughts behind the

technology selection. Since the overall goal is to reduce carbon emission is the most logical and reasonable choice to produce the hydrogen in such manners so that the CO2 emissions are not negatively affected. What highly contributed to the selection of reforming technology was the construction of water electrolysis at Herøya Industry Park, close to the INEOS production plant [58, 59].The water electrolysis splits water into hydrogen and oxygen by the means of electricity. This can open the opportunity of purchasing oxygen at a lower price since it is a by-product. This again opens the opportunity of operating systems that has oxygen as an input at a lower cost than firstly assumed.

Another important consideration revolves around the readiness for implementation. If the decarbonization of the ethylene production at INEOS is happening in near future should the technology selection emphasize the maturity of the system that are to be implemented. With this in mind was several of the technologies described in the previous section taken out of the equation. Left was the mature hydrogen production methods, such as SMR, SMR+, POX, CPO, and ATR. The SMR and the SMR+ system involves an emission which is quite higher than for example the ATR. This difference is mainly caused by the need for external heat, which is traditionally supplied by combustion of fossil fuels. Another aspect related to emission is that the size of the reformer and a SMR is undoubtedly larger. [43] The electric reformer is definitely an interesting option with potential but are not commercially available yet. In addition is the realization of water electrolysis with oxygen as a secondary product close to the production site made the systems based on partial oxidation particularly interesting. Since the major drawback of these systems is an expensive oxygen production unit (around 40% of the investment of a syngas production system), can it be reasonable to assume that the system will be more advantageous if this expense if reduced. The system relevant was consideration is therefore POX, CPO, and ATR. The preferred technologies for production of hydrogen at a very large scale does not include the CPO. This is mainly because the upscaling of inlet mix presents some challenges, and the oxygen consumption exceeds the ATR. If the system were for a small to intermediate scale would the CPO be more attractive because of its compactness. The oxygen consumption for the POX is also exceeds ATR mainly because the inlet temperature of the ATR traditionally is higher (650°C compared to 250°C). Since the outlet temperature are approximately equal for the POX and the ATR for the same conversion rates will the POX require more oxygen to cover the gap in temperature. [50] Taken this into consideration was the conclusion of the technology selection an ATR system.

5 Introducing Aspen HYSYS and presentation of base case

This chapter presents the general inputs and assumption to Aspen HYSYS, as well as the simulation of base case. The first section includes a more detailed problem description. The second section presents an introduction to Aspen HYSYS. The third section presents input, assumption, and simplifications in Aspen HYSYS. Lastly, in the fourth section is the presentation of the base case.

5.1 Detailed problem description

Fuel substitution was briefly presented in section 3.3. To elaborate will a simplified energy demand for a system be presented. A production plant, for example INEOS, produces 650 000 ton ethylene annualy by using 12 cracking furnaces, with an inlet flow of 150ton/h ethane. It has an energy demand both to the cracking furnace and to the following separation process. In this report is it only considered the replacement of the energy supplied to the cracking furnace by combustion, since this is the main area of interest for this feasibility study. The cracking furnaces gets the fuel for combustion from the cracker outlet, more specifically the hydrogen and the methane. In the separation process is this taken out and fed back to the furnace and combusted with air. If this fuel are to be substituted with only hydrogen is it important that the energy supply is minimum equivalent, if maintaining the same production rate of. The inlet flow to the reforming process is calculated from the oulet flow of the cracker and it is assumed that all methane and hydrogen is used as fuel. Under this assumption amounts the flow to 8250kg/h CH4 and 6000kg/h H2, given that 5.5wt% and 4.0wt% of the inlet flow becomes CH4 and H2, respectively. [10]

The purpose and the main goal of this project is to investegate if reformation of methane to hydrogen, and use this as a fuel replacement in the cracking furnace, is a viable solution. If it appears as a feasible solution after this initial study, may the project be taken to the next step. This process solution potentially reduces the carbon footprint and reduce the number of CO2 capture points, compared to capturing it at all the different furnace flue gas points. To complete this and to quantify the different energy demands, temperatures, pressures, flowrates, and compositions, the overall process will be simulated in Aspen HYSYS. The base case (Case 0) have a traditional setup presented in section 5.4, and four different configurations (Case 1-4) are tested and described in chapter 6. The affect of variating the most important parameters are studied and presented in section 7.1. The results is used to suggest a system with improved preformance (Case 5) in 7.3. The improved case are investegated for potential steam import or export, and a suggested MER-network design are presented in section 8.2 and 8.3. The system is evaluated and discussed in chapter 9.

5.2 Introduction to Aspen Hysys

In 1977 started the advanced system for process engineering (ASPEN) project, where the main goal was to develop a simulation tool that could be used across a variety of industries. This project would over the next years and decades evolved to become AspenTech, a global

industry-leading software for process design, simulation, and optimization. [60] Aspen HYSYS is a branch in AspenTech. Because of Aspen HYSYS' high innovation factor and process simulation accuracy, was the software given the title of "Best Modeling Technology" at the 2020 Hydrocarbon Processing Awards. [61] These accomplishments, along with the availability and the task description, was the preferred simulation program obvious.

5.3 Input, assumptions, and simplifications in the Aspen HYSYS simulations

The input to the simulations for all the cases (Case 0 to Case 4) has similarities in the input, assumptions, and simplifications. The effect of these will, to some degree, be discussed and evaluated in chapter 9. The primary goal of this study, as mentioned previously, is to investigate the applicability and possibility of implementing a reforming system for substitution of the current fuel to a cracking furnace. Since this is an initial step towards a possible implementation is the required accuracy somewhat lowered but should be within reasonable limits.

The specifications and input to the simulation is based on or inspired of several previous studies and literature [8, 50, 62-64]. Additionally, some input has been based on assumptions and simplifications within acceptable limits as far as to the knowledge of the author goes.

The inlet stream is assumed to not have contaminations (for example sulfur), meaning there is no need for a purification unit prior to the process. The water used in such system tend to be demineralized (removed of salts) but that is not considered. All the simulations use the Peng Robinson equation of state, and the components involved in every simulation is chosen. The pressure-drop over every heat exchanger is set to 10kPa and there is assumed not to be a pressure drop in the reactors. There is also assumed no heat loss in the system and the adiabatic efficiency of the compressor is 75%. All the reactors are simulated as Gibbs reactors (minimizing the Gibbs free energy) and presumed to be accurate enough. When simulating the system, it is required to specify a liquid outlet stream of the reactors. These streams have no flows but is represented with a normal material stream arrow. To avoid confusion has the liquid outlet streams of the reactors no name nor a following attachment in the snapshots, making it easier to differentiate between the flows that are empty and not. There also assumed to be no build-up in the system.

The initial separation step is suggested to be a membrane that separates out 95mol% of the inlet hydrogen prior to the reforming system to a purity of 100% (assumed). This is simulated as a component splitter. The component splitter is also used when simulating the CO2 separation and the H2 purification. This is a simplification, and the parameters are assumed. The component splitters are merely to exemplify the possibility of different separation steps.

The detail of all simulations is found in the tables available in Appendix B. The base case is described with the most essential parameters and properties, and the following cases originates from this. The alterations are described, along with the most important numbers. However, the details such as molar flows and compositions, temperatures, and pressures can be found in the corresponding table in the Appendix B.

5.4 Case 0: Process simulation and description of base case

The concept of an ATR was described in section 4.2.4. This section presents the base case simulation of the ATR process. A snapshot from Aspen HYSYS is presented in Figure 5.1, where the major streams and components are named. The feed to the system is "Inlet flow, CH4 and H2" with a flow rate of 514.2kmole/h CH4 and 2976.3kmole/h H2. This is fed into a membrane where 95mol% of the H2 is separated out and sent directly to the burner. The retentate side of the membrane is mixed with steam in a ST/C ratio of 1.62 and compressed to 2300kPa. The compressed flow is heated to a temperature of 650°C before entering the ATR. O2 is added to the ATR in a O2/C ratio of 0.6, and the occurring reactions are highly exothermic, eliminating the need of external energy. The temperature the ATR outlet is 1050°C and the stream is partly utilized to heat the inlet flow to the ATR. The outlet of the ATR is cooled before being fed to two WGS reactors. One high temperature water-gas-shift (HT-WGS) and one low temperature water-gas-shift (LT-WGS) with the inlet temperature of 300°C and 175°C, respectively. The WGS reaction is slightly exothermic, and the process stream must be cooled both before and after the reactors. After the WGS reactors follows two separation processes simulated as component splitters. The first separates out 90mol% of the CO2 to a purity of 99.55mol% and the second one separates out 90mol% of the H2 to a purity of 96.8mol%. These numbers are assumed, and the separation steps can, for example, be chemical absorption and PSA. The two flows of hydrogen are sent to a burner. The combustion receives stoichiometric amount of air, and the outlet stream of the burner is mainly water and nitrogen. The energy released from the combustion process ("Burner" in Figure 5.1) is representing the energy supplied to the steam cracking furnace.
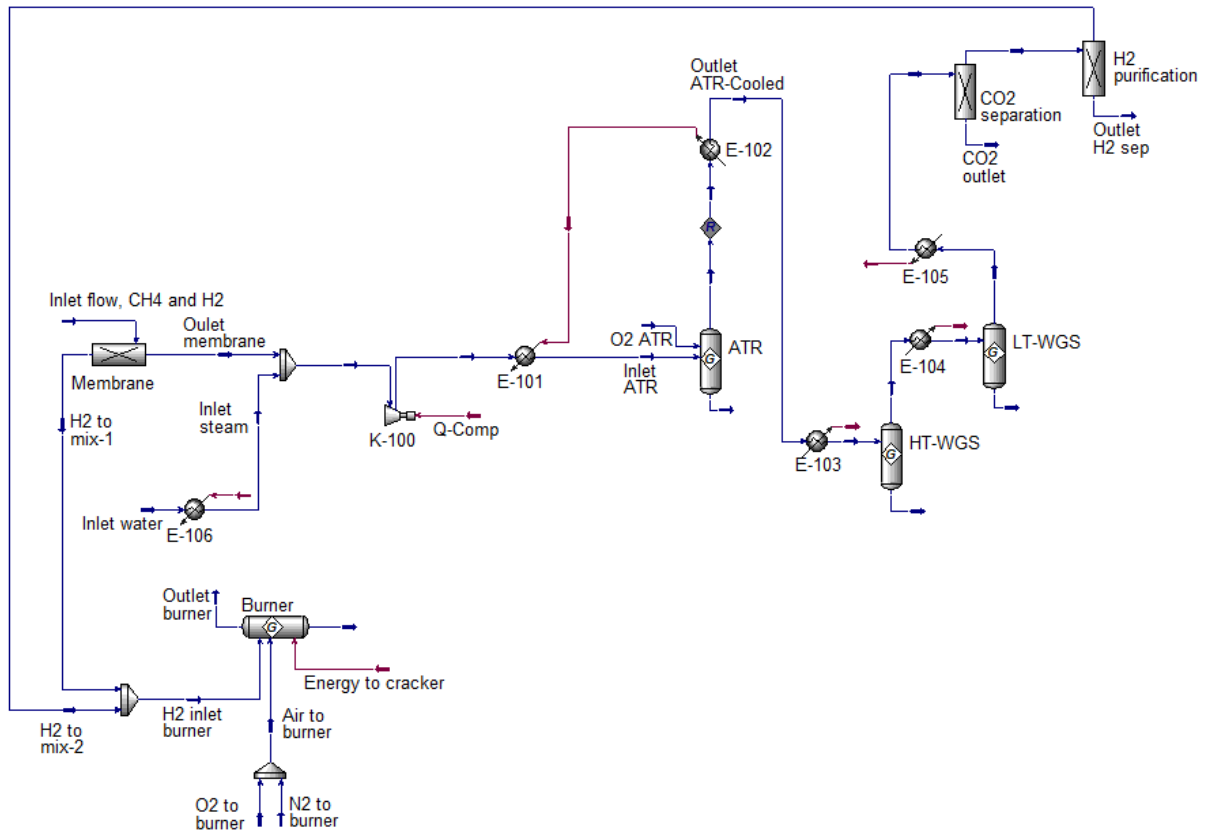
Figure 5.1 Snapshot from Aspen HYSYS of Case 0 (base case)

6 Simulation and modification of an ATR process in Aspen HYSYS

This chapter presents the simulation and modifications of the ATR system in Aspen HYSYS. The first section includes a comparison of the energy content from combustion of pure H2 with combustion of a mix of H2 and CH4. Each of the following four sections includes one configuration that separates it from the base case.

6.1 Comparing burners with different fuels in Aspen HYSYS

The main goal of this project is to investigate if there are enough energy to cover the requirement of a steam cracker. The natural starting point is to detemine how much hydrogen is the minimum to keep the same production rate of ethylene. The current energy supply is combustion of the methane and the hydrogen that are products of the cracker. To repeat, is it assumed that the amount of methane and hydrogen that is burned is the total amount of these components exiting the cracker. A typical amount is aound 5.5wt% CH4 and 4.0wt% H2 in the exit gas of the cracking furnace [65]. This is in the same range as standard steam cracker for ethylene production with ethane as feed [10] and is therefore assumed to be comparable with the actual composition at INEOS. An inlet flow of 150 ton ethane per hour will result in a flow of 514.2kmole/h CH4 and 2976.3kmole/h H2 on a molar basis. To simplify and to make the comparison on the same terms is two burners simulated in Aspen HYSYS, Burner 1 and Burner 2. Burner 1 has pure hydrogen (100mole%) as fuel and Burner 2 has a mix of hydrogen (0.1473mole%) and methane (0.8527mole%) as fuel. Both is combusted in air with a flow rate that gives 100% conversion of the fuel, and both burners has the same inlet and outlet pressure and temperature. Burner 1 has a flow rate of 4231kmole/h, corresponding to the flow of hydrogen that enters the burner after reformation in Case 0 (base case). Burner 2 has a flow rate of 3491kmole/h, corresponding to the flow of methane and hydrogen that exits the steam cracker (and is the inflow to the reforming process). The snapshot of the simulated burners are illustrated in Figure 6.1. Burner 1 and Burner 2 has a heat flow of -6.935e+008kJ/h (Q1) and -7.478+008kJ/h (Q), respectively. The negative sign indicating that heat is going out.
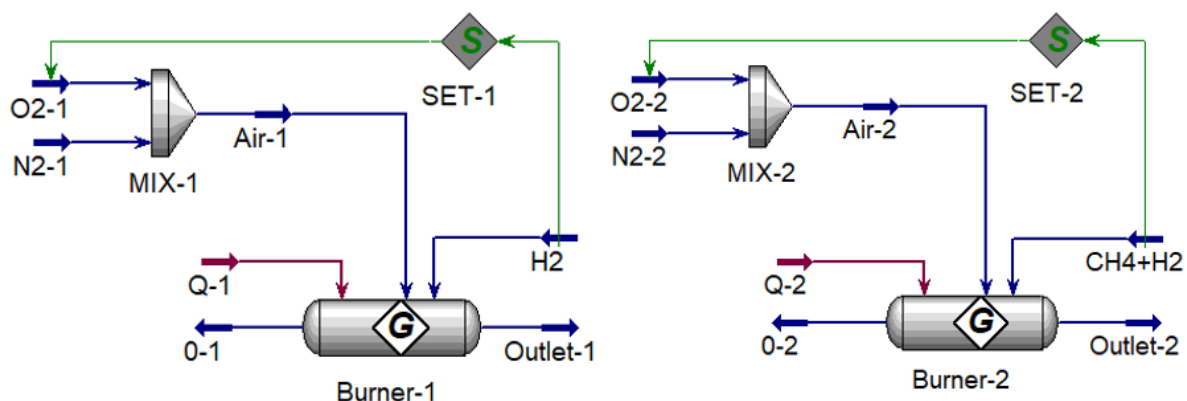
Figure 6.1 Snapshot from Aspen HYSYS simulation of burners. Left is Burner 1 and right is Burner 2.

When comparing the heat flows of Burner 1 and Burner 2 (having in mind that this should supply energy to the cracker) it implies that the base case does not have a high enough energy to supply the cracker furnace. If the inflow of hydrogen to Burner 1 is increased until the heat flow from Burner 1 matches or exceeds the heat flow from Burner 2, the result is a hydrogen flow of 4565kmole/h. This elevated flow of hydrogen results in an energy flow of -7.482e+008kJ/h, which is slightly above what is required. This means that more hydrogen than what is produced in the base case is necessary. This is a simple approach to set a goal and requirement for further development of the process. And as mentioned, is this only for comparison reasons. The details and the stream properties can be found in Appendix C.

6.2 Case 1: Process description of implementation of recirculation stream

Case 1 has all the equal input parameters as Case 0 with one exception. The gas exiting the H2 purification unit is recycled back and enters along with the steam prior to compression. The stream consists of approximately 60mol% H_2O, 27mol% H_2, 1mol% CO_2 and minor amount of CO and unconverted CH_4. The flow amounts to 624.4kmole/h. Recycling of this stream leads to a few observations. One being the reduced flow of inlet water, from 835 to 450.6kmole/h, while remaining the ST/C ratio of 1.62. This is due to the content of water in the recycle. This will also result in a lower temperature in the ATR outlet which generally relates to lower conversion of methane. This can be seen from the increased flow of methane, from approximately 3 to 12kmole/h. This can be compensated for by increasing the inlet temperature of the inlet flow(s) or increase the flow of oxygen. An optimization of the process is not completed at this stage for this case. The process flow in the system from the compressor and for all following units is increased, and the result is a need for equipment and vessels with higher capacity and therefore higher cost. However, valuable H2 will be fed back into the system causing the overall hydrogen production to increase. It will from this point on be assumed that such a recycle brings more advantages than disadvantages and the recycle kept attached when simulating the other cases. The most important result from the simulation is the energy from the cracker, and the absolute value has increased to -7.201e+008kJ/h (compared to -6.911e+008kJ/h in Case 0). Still, lower than the amount required to maintain today's ethylene production. Figure 6.2 is a snapshot of the simulation.
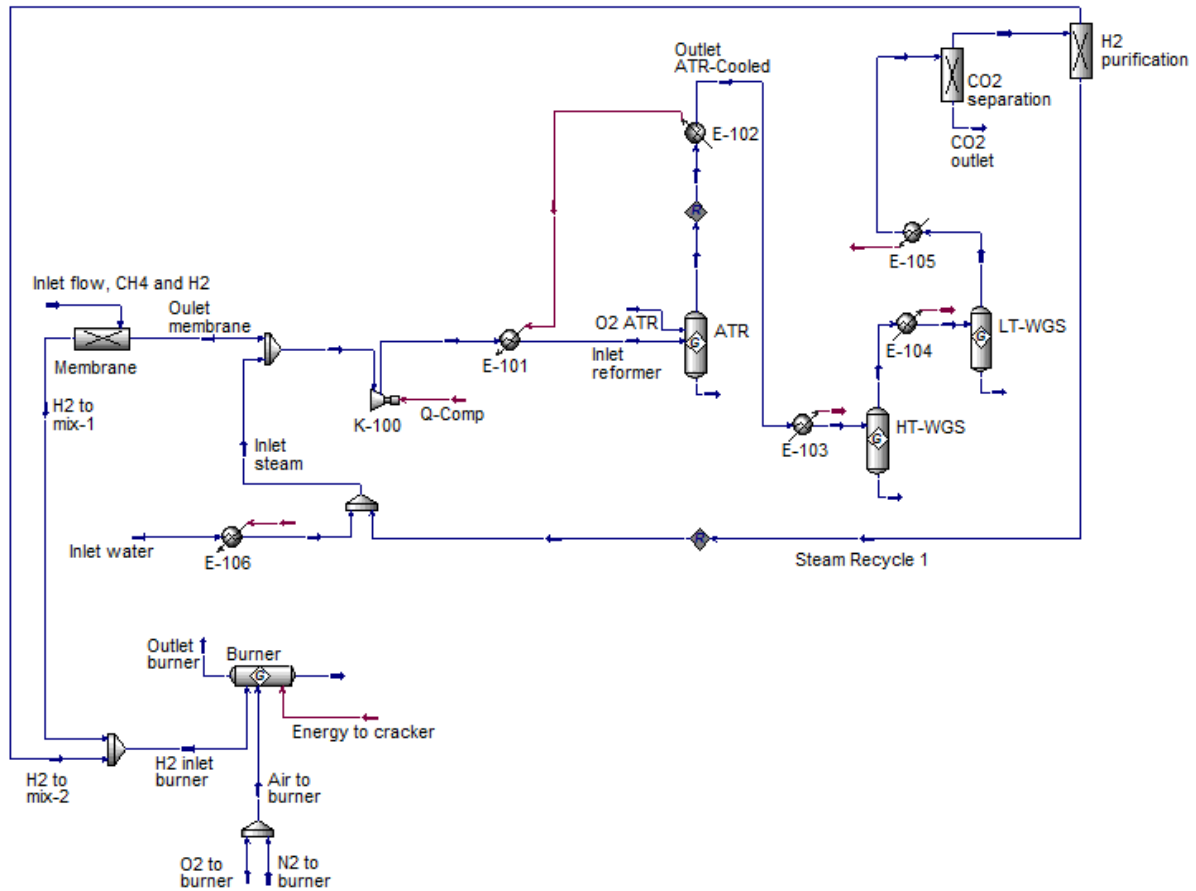
Figure 6.2 Snapshot from Aspen HYSYS of Case 1 (implementing a recycle)

6.3 Case 2: Process description of implementing an extra inlet stream (of ethane) to the system

Neither Case 0 nor Case 1 fulfilled the required amount of hydrogen to satisfy the desired energy supply. There are multiple approaches to increase the amount of hydrogen to the burner. The chosen approach was to have an additional inflow of ethane to the reforming system. The ethane is assumed to be available on site or easy to purchase since this is the raw material to the cracker. More specifically, the ethane is added between the membrane and the compressor, together with the recycle stream. The ethane flow was adjusted until the desired flow of hydrogen to the burner was reached. Note that this both increases the steam and oxygen consumption, as discussed in the following chapters. If all ratios, temperatures, and pressures from base case are kept constant, and only the inflow of ethane is adjusted, amounts the ethane flow to approximately 40kmole/h.

The input to the simulation is the same as Case 1 with the change of adding ethane. The configuration is referred to as Case 3 and a snapshot of the simulated process are presented in Figure 6.3. If the ST/C and O2/C ratio are kept constant (1.62 and 0.6), must the inlet flow of steam and oxygen be increased. The outlet temperature of the ATR is slightly lower than Case 0 (1032 compared to 1050℃). The conversion of methane is a little lower compared to Case

0, but the amount of produced hydrogen is increased. The flow of hydrogen to the burner is increased from 4231.2 to 4587.5kmole/h which results in more energy. The energy that can be supplied to the cracking furnace amounts to -7.503e+008kJ/h, slightly above the minimum.
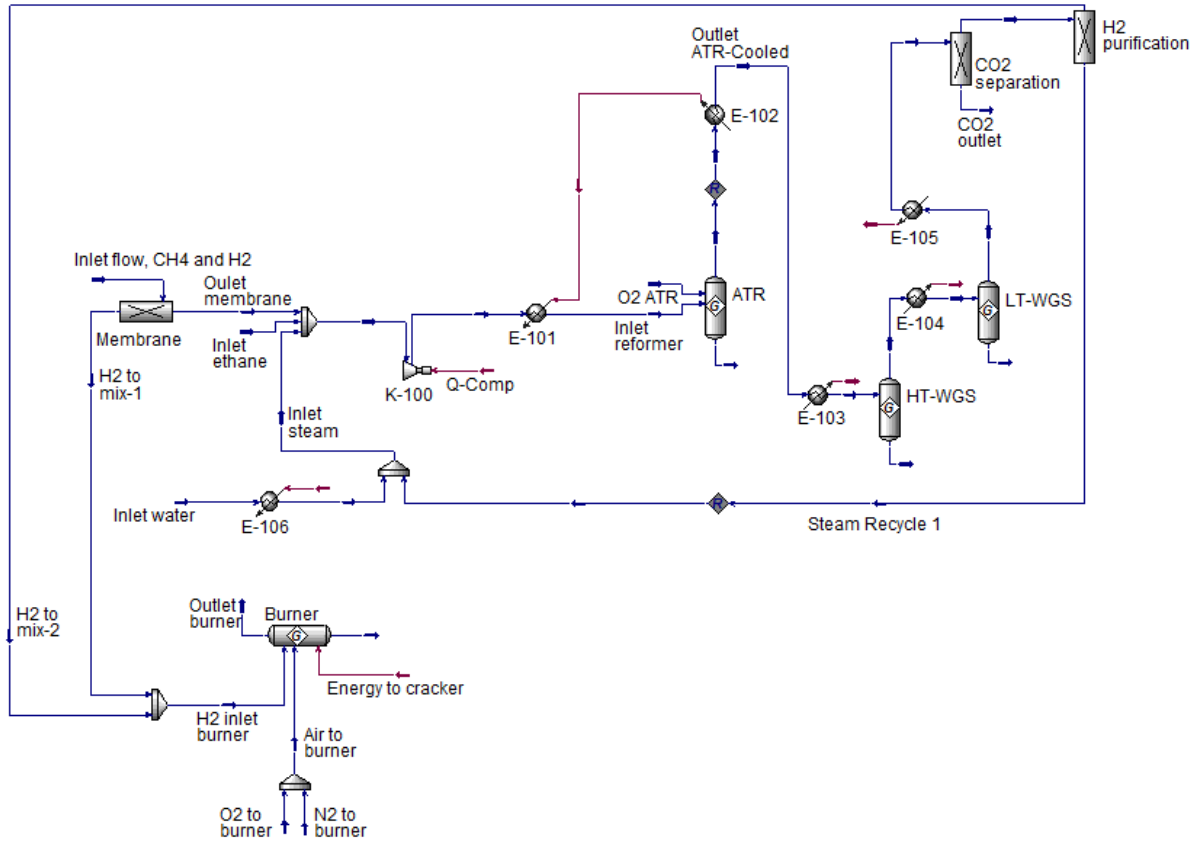
Figure 6.3 Snapshot from Aspen HYSYS of Case 2 (adding ethane to the process)

6.4 Case 3: Process description of adding CO2 to the ATR

The main advantage of the ATR process is its self-supply of thermal energy. However, there are some challenges related to this reforming method as well. The temperature in the reactor may exceed the limits of the material and/or lead to total combustion. In the previous cases (Case 0, Case 1, and Case 2) was this temperature altered by selecting an appropriate ST/C and O2/C ratio. More steam or less oxygen leads to a lower temperature and vis versa. The optimum is a tradeoff between conversion, consumption, and cost, but that is not pursued here. Reforming by CO2 is referred to as dry reforming and has received some attention in literature, both encouraging and constructive. There has been conducted tests on pilot scale [50] but not with outstanding results. It is in this work regarded as an unfavorable option compared to other methods available [47]. In despite of this, is it chosen to add a CO2 flow as an example. The flow of CO2 might also serve as a temperature regulation of the ATR outlet temperature. This was for Case 3 chosen to be CO2, mainly because this would be present at the plant site. Seen in retrospect may other options be more favorable since the adding of CO2 can enhance the reverse WGS and temperature adjustment can be done by other means, such as adding H2O.

The input to Case 3 resembles Case 1, but with two alterations. One alteration is the inflow of CO_2 to the ATR. The second is the steam input. To demonstrate the effect of the CO_2 is the ST/C ratio decreased to 1.0 (from 1.62) which leads to an increased temperature in the ATR outlet. Without the inflow of CO_2 would the temperature become 1100°C (from 1050°C in Case 0), and with a flow of 75kmole/h CO_2 would it degrease again to 1050°C. The CO_2 input parameters was chosen in the same range as the outlet of the CO_2 separation unit. Temperature of 200°C and pressure of 2290kPa (where all is assumed). A snapshot for the Aspen HYSYS simulation is presented in Figure 6.4.
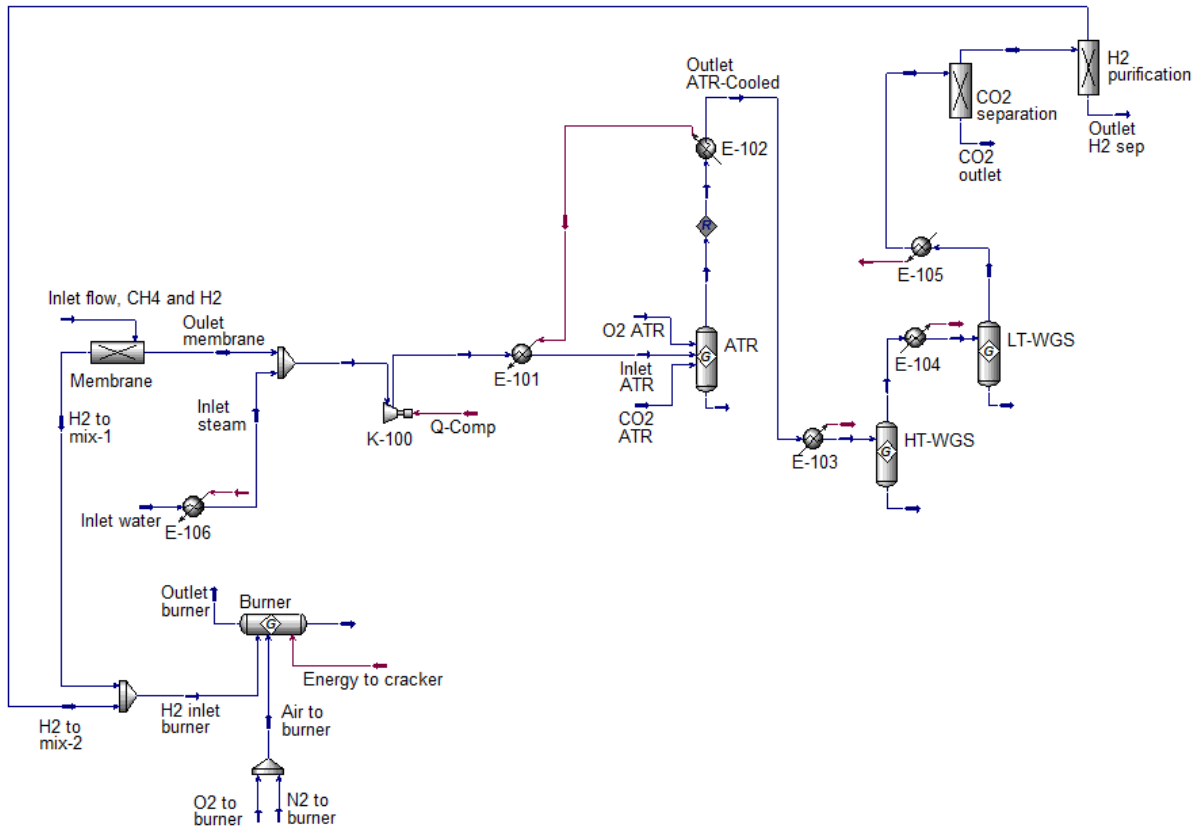
Figure 6.4 Snapshot from Aspen HYSYS of Case 3 (adding CO_2 to ATR)

The main disadvantage of choosing CO_2 for lowering the temperature is that the CO_2 might react with the H_2, producing CO and H_2O (the reverse WGS reaction). This is the reverse of the WGS reactions that are desired in the downstream process steps. Meaning that the CO_2 might counteract the hydrogen production, causing lowered conversion rates in the HT- and LT-WGS reactors.

6.5 Case 4: Process description of replacing HT- and LT-WGS with MT-WGS

The traditional setup of a reforming process for hydrogen production is implementation of two WGS reactions downstream of the reformer. This is to produce more H_2 and CO_2 from CO and H_2O. Advances in the catalyst stability and activity has made the MT-WGS a more reasonable option than previously.

Replacing two reactors of high and low temperature with one medium temperature reactor has obvious advantages, considering the reduction in number of units. In regard to hydrogen production is a MT-WGS reactor an attractive solution, because it potentially reduces the required steam to the process. The medium temperature reactor operates in a higher temperature range than the HT- and LT-WGS reactors. This has made is more challenging to develop a catalyst which function adequately in the whole interval, being both active in the lower region and stable in the higher region. However, the advances in catalyst technology have made the MT-WGS the preferred solution when it comes to producing hydrogen. [8]

A snapshot of the Aspen HYSYS simulation is presented in Figure 6.5. The input parameters resemble Case 1 apart from the WGS reactor. The HT- and LT-WGS reactors with an inlet temperature of 300°C and 175°C, respectively, has been replaced by a MT-WGS reactor with an inlet temperature of 225°C. The outlet temperature increases to 366°C.This is an increase of 141°C compared with the increase in HT and LT in Case 0 of 121.8 and 45.3°C, respectively.
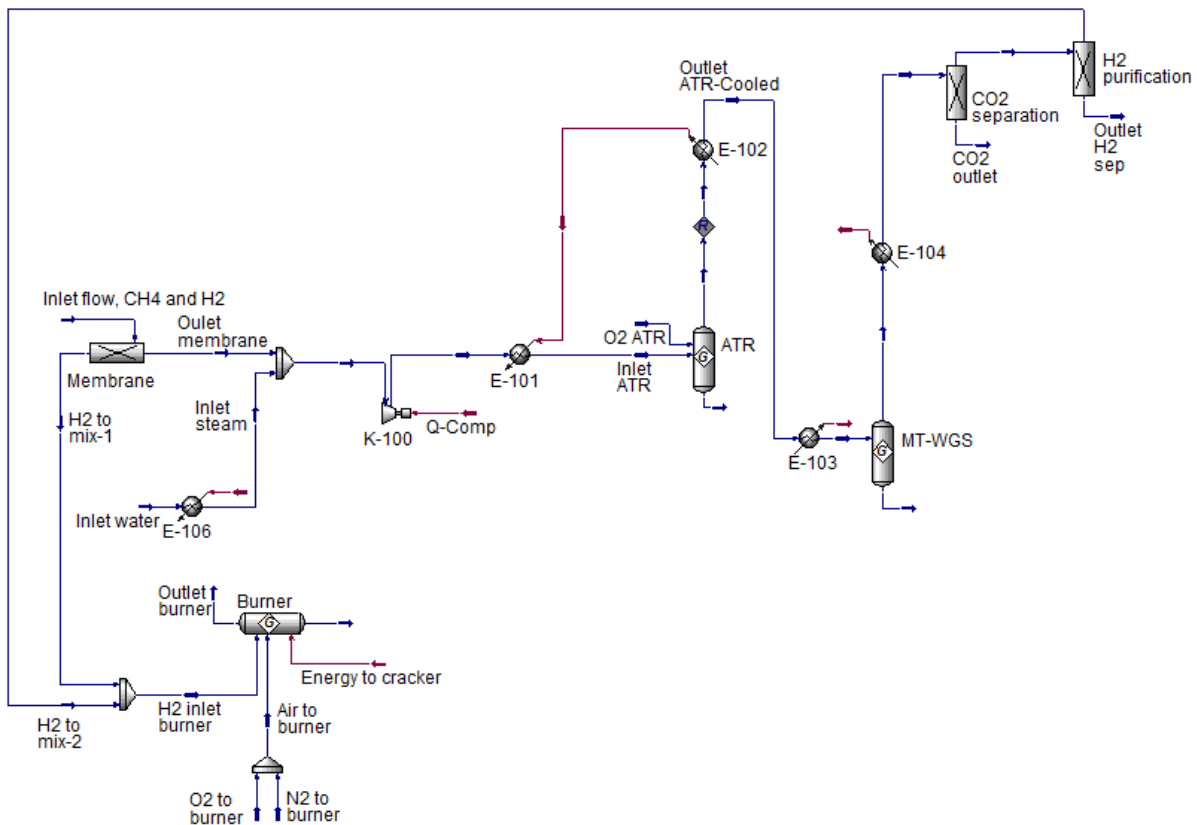
Figure 6.5 Snapshot from Aspen HYSYS of Case 4 (with MT-WGS)

The production of hydrogen is lowered to 4177kmole/h compared to 4231kmole/h in Case 0. Resulting in an energy to the cracker of -6.820e+008kJ/h. However, the difference in hydrogen production (and therefore energy) may be lowered for an optimized system. A possibility for using a MT-WGS reactor while reaching the hydrogen production target is to add an additional flow of ethane to this system as well.

7 Analyzation and evaluation of the simulated systems

This chapter presents the analyzation and evaluation of the simulated systems (Case 0-4). The first section includes case studies in Aspen HYSYS where several parameters is variated. The second section an evaluation for the different configurations and parameters. The third section presents a partly optimized process for maximizing hydrogen production.

7.1 Case studies

Case studies in Aspen HYSYS is a method that can be used to analyze the effect of a parameter. This is done by choosing an independent variable which is varied within a chosen interval, and with a chosen step size. The dependent variables of interest are selected and there is only one independent variable that varies at the time. Aspen HYSYS provides the results both in both tables and plots. Appendix D includes the tabulated results from the case studies. The results of the flow the total flow of hydrogen and CO2 is summarized in the end for all the case studies, in section 7.1.4.

7.1.1 Case studies for Case 2

This section will only present the input and results of the case studies conducted for the process conditions of Case 2. The. The evaluation and thoughts on selecting optimal conditions will be given in section 7.2 and 7.3. Note that the recycle is not attached during the case studies.

7.1.1.1 Steam-to-carbon ratio (ST/C)

Adding steam to a reformation process (such as this one) has two main goals. The first one is the increase in hydrogen production and the second one is the prohibition of soot formation. The ST/C is normally between 1.0 and 2.0 for an ATR and can increase beyond for feedstock with heavier hydrocarbons. An increase in the ST/C ratio should cause an increase in hydrogen production and decrease CO production. [8]

The case study variated the ST/C ratio from 0.5 to 5.0. Corresponding to an inlet flow of water in the range of 300 to 3000kmole/h. The result was that increased ratio led to a decrease in the outlet temperature of the ATR. Not surprisingly did it also lead to an increase in the energy stream to the heat exchanger prior to the ATR (E-102), because of a higher flow. The outlet molar composition flow of H2, H2O and CO2 increased, while for CO it decreased. The flow of CH4 and C2H6 only changed minorly, while the O2 remained at zero.

7.1.1.2 Oxygen-to-carbon ratio (O2/C)

The case study has a O2/C ratio from 0.2 to 1.0, corresponding to 120 to 600kmole/h of O2. This ratio should be one of the last parameters to be optimized due to the fact that it depends on the pressure, temperature and the ST/C ratio.[66] Too much oxygen could also lead to total combustion which will result in a lower hydrogen production and temperature beyond what the material can withstand.

The increase in the O2/C ratio gave an increase in the outlet temperature of the ATR (725 to 1936°C). The energy stream to the heat to E-102 remained constant because the identical flow was risen to the identical temperature throughout the case study. The outlet molar composition changes after all the CH4 are consumed. This happened at an O2 flow of 375kmole/h (which is a O2/C ratio of 0.635). Until that point (and a little further) is there an increase in CO and a decrease in CO2. Hydrogen reaches its highest fraction when the flow of O2 is at 315kmole/h (which is a O2/C ratio of 0.53). The composition of H2O decreases until it turns at right before the flow of O2 reached 300kmole/h.

7.1.1.3 Pressure in ATR

The case study for the pressure in the ATR was conducted by cloning the ATR in the Case 2 and complete this study without the upstream and downstream part. The hydrogen production is favored at lower pressure as can be seen from the occurring set of reactions where there is an increase in the number of molecules. The normal range in pressure are between 2000 and 10000kPa and higher pressures requires higher temperatures for the same conversion of methane. [8] Another important factor when designing the ATR and determining the pressure is the separation and utilization after the ATR. If this separation is at a higher pressure can it be favorable with a higher pressure in the ATR and vis versa if the downstream separation has a lower pressure [62].

The case study involves a pressure from 2000 to 10000kPa. The result was that an increase in pressure gave an increase in temperature. The outlet molar composition has less H2 and CO and more H2O. CH4 increased minorly and CO2 degreased minorly.

7.1.1.4 Temperature of the oxygen to the ATR

The case study for the temperature of the oxygen to the ATR was in the interval of 20 to 750°C. The increase in temperature of O2 also increased the outlet temperature of the ATR, as predicted (from 1050 to 1161°C). This caused the outlet molar composition of have more CO and less CO2. Slight increase in the H2O content and decrease in H2, while CH4 did not change substantially, and the oxygen and ethane remained unchanged.

7.1.1.5 Temperature for the HT-WGS and LT-WGS

The catalysts utilized in WGS reactor are temperature sensitive. The equilibrium constant clearly favors a low temperature at the inlet, but the catalysts has traditionally not been active until a higher temperature is reached (above approximately 330°C). Even if there are possibilities below this temperature are the catalyst usually sensitive to contamination. Another limitation is the condensation of the inlet, so this must be carefully be monitored if a temperature close to the dew point is selected. [8] There have been improvements is this area lately and one can only assume that the development will continue. These improvements along with the assumption of a flow with no contaminations is the inlet temperatures in the lower part of the region.

The case study for the inlet temperature for the HT-WGS was conducted between 250 and 450°C. Not surprisingly did the outlet temperature increase along with the inlet temperature. It also showed that outlet molar composition increased in CO and H2O and decreased in CO2 and H2. CH4 (inert), C2H6 (inert) and O2 remained constant. The molar H2/CO ratio in the outlet got lower when the temperature got higher with 13.3 at 300°C and 10.7 at 350°C. [8]

The same trend lines can be observed when increasing the inlet temperature for the LT-WGS in the range from 150C to 250°C. The H2/CO ratio decreased from 14.1 at 175°C to 95.2 at 200°C.

7.1.1.6   Flow of O2 to the burner

The case study varies the flow of oxygen (and nitrogen follows thereafter) from 1000 to 3000kmole/h. Heat is released and is representing the energy supply to the ethane cracking furnace, meaning that the highest absolute value of the heat flow is desired. This value is at 2201kmole/h of oxygen, in the case study this is exactly stoichiometrically (note that there is a slight deviation between this value and the one in Case 2, this is because of the recycle which is not attached causing some minor changes). Before the amount reaches the stoichiometric amount is there a descending flow of H2 and CO. When the flow surpasses the stoichiometric amount of O2 is the H2 and CO stable at zero, while the molar composition of CO2 and H2O decreases and oxygen increases.

7.1.1.7   Temperature inlet of the ATR

The case study varies the temperature into the ATR in the range of 600 to 800°C. Increased temperature leads naturally to a higher heat flow to the heat exchanger before the reformer. Keeping all other variables constant is it observed that increased temperature leads to increased CO and H2O composition in the ATR outlet, and a decrease for H2 and CO2. This might appear unfavorable but increase in CO results in higher possible conversion in the following WGS reactors. The overall molar flow of the hydrogen increases.

7.1.2   Case studies for Case 3

7.1.2.1   Flow of CO2 to the ATR

The flow of CO2 to the ATR is primarily a way to adjust the temperature in the reactor but also a way to increase the CO in the outlet, which may be advantageous for some applications. A flow of CO2 can prevent carbon formation at lower ST/C-ratios [8] or in some cases increase the risk for soot formation [50]. The flow was in Case 3 of 75kmole/h which gave an outlet temperature of 1050°C. The case study involved flow rates from 0 to 20kmole/h and as predicted did the increase in CO2 flow cause a decrease in the outlet temperature (1100 to 987°C in the given interval). The CO, CO2, H2O and CH4 content increased while the H2 decreased.

7.1.3   Case studies for Case 4

7.1.3.1   Temperature for the MT-WGS

The case study for the inlet temperature for the MT-WGS was conducted between 150 and 250°C. Not surprisingly did the same trendlines as for the HT and LT-WGS reactors observed. One factor to take note of is that the vapor fraction in the inlet did not reach 1 until a temperature of 165°C, meaning that this is the lower limit. The result was that outlet molar composition increased in CO and H2O and decreased in CO2 and H2. CH4 (inert), C2H6 (inert) and O2

remained constant. The molar H2/CO ratio in the outlet got lower when the temperature got higher with 25.5 at 200℃ and 21.0 at 225℃. This result corresponds with literature.

7.1.4 Summary of case studies

Table 7.1 summarizes the effect on outlet flow of CO2 and the overall H2 production. The base case simulation had a molar flow of 524kmole/h of CO2 and 4450kmole/h of H2. The numbers presented in the table is in a range, representing the lowest and highest values achieved within the limits used in the corresponding case study and again is the recycle not attach. The pressure in the ATR was analyzed by cloning the reactor in Aspen HYSYS, eliminating the possibility to see the CO2 and H2 molar flow rates directly. The interval given in the table is therefore the minimum and maximum found when manually testing various pressures in the interval of 100 to 5000kPa.

Table 7.1 Summary of CO2 outlet flow and H2 production for the various case studies

	CO2 outlet flow [kmole/h]	H2 production [kmole/h]	Note/Trendline
ST/C-ratio	361.3 – 535.7	4258 - 4614	Higher ratio results in higher CO2 and H2 molar flows
O2/C-ratio	235.1 – 534.1	3747 - 4464	Higher ratios result in higher CO2. H2 production peaks when O2/C is 0.57
Inlet temperature HT- and LT-WGS	HT: 526.0 - 516.3 LT: 504.5 – 528.0	HT: 4444 – 4451 LT: 4434 - 4453	Increasing temperature results in degreasing flows of CO2 and H2
Inlet temperature MT-WGS	386.9 - 419.9	4227 – 4252	Increasing temperature results in degreasing flows of CO2 and H2
Pressure ATR	522.7 - 525.8	4432 - 4457	Increasing pressure results in degreasing flow of CO2 and H2
Inlet temperature ATR	523.0 – 525.0	4445 - 4455	Increasing temperature results in increase in flow of CO2 and H2

Inlet temperature of O2 to ATR	524.0 – 524.9	4450 - 4454	Increasing temperature results in slightly increase in flow of CO2 and H2
Flow of CO2 to ATR	420.4 – 581.4	4182 - 4222	Increasing flow results in increase in flow of CO2 and decrease in flow of H2

As can be seen from Table 7.1 is hydrogen production favored at high ST/C ratio, O2/C ratio of 0.57, low inlet temperatures to the WGS reactors, low pressure, low flow of CO2 and high temperature in the ATR. A 'perfect' system has minimum amount of CO2 produced and maximum amount of H2 produced.

7.2 Evaluation and selection of optimal operating conditions

The most important output is the simulated/assumed energy requirement for the ethane steam cracking furnace. Case 2 has enough energy to meet this requirement. However, it is highly advantageous that the process operates economically, in a sense that consumption of ethane and oxygen is at minimum, as this is purchased. Lowering the consumption will potentially lower the operational cost. The increase in flow throughout the system will also be a determining factor when sizing the equipment, which will affect the investment cost. So, there will be a tradeoff between efficiency, amount produced, operational cost, and capital cost.

The case studies showed and confirmed several trend lines for different parameter variations. The selection of optimal operation conditions in an overall sense is not possible to complete properly when the cost is not a part of the equation and only one parameter is evaluated at the time. Nevertheless, there are some parameters that are more advantageous to promote than others. For starters is maximum methane and ethane conversion important, as well as maximum hydrogen production and the flow of CO2. Other parameters that may also be of significance is the possibility of steam export.

This system will by no means be completely optimized, neither for production or conversion, nor for cost. This is a feasibility study and an investigation of the possibility to implement a reforming process for a cracking production plant, such as INEOS. The focus will therefore be on high hydrogen production. But there are some advantages and disadvantages related to all the cases described and the main ones are summarized in Table 7.2.

Table 7.2 Main advantages and disadvantages for the simulated cases (Case 0 - 4)

	Main advantages	**Main disadvantages**
Case 0	Lowest complexity	Does not produce enough H2 Low utilization of resources

Case 1	Increased utilization of resources Higher H2 production (less lost)	Does not produce enough H2
Case 2	Produce enough hydrogen	Higher flow throughout the system
Case 3	Produce enough hydrogen Easier temperature control	Lower conversion
Case 4	One less reactor and heat exchanger	Lower H2 production (but can be compensated with ethane inflow) Higher flow throughout the system

From Table 7.1 and Table 7.2 can it be seen that some choices for further work is more appealing than others. Case 2 and 4 is the ones that overall comes out on the winning side of the selection. Both may accomplish a satisfactory production of hydrogen, both consists of well testes technologies that are ready for implementation, and both have potential for further optimization along with their possible steam export. The hydrogen production is likely to increase when optimal conditions are chosen if the cost does not hindrance it. If the produced hydrogen exceeds the desired rate can this be adjusted by reducing the amount of ethane fed to the system. As will be discussed in chapter 9 is this by no means a system without uncertainties and assumptions, and further development and investigation must be completed before the level of accuracy raises.

To summarize in words what favors conversion of hydrocarbons and production of hydrogen it is the following points (seen from the simulations, case studies, and literature research). The trend lines that are seen is in agreement with previous studies. [50-52, 62, 66]

- Low pressure. It should be at the lowest as possible and is generally limited by the downstream purification steps, the volumetric flow through the system (which affect the dimensions), and carbon formation.
- High temperatures, both in the inlet and outlet of the ATR. Generally limited by the material and the risk of total combustion.
- High ST/C ratio. The steam contributes to higher hydrogen production, as well as prohibition for coke formation. The downside is increases energy requirement (because the temperature drops with an increase of steam) and the flow through the system.
- O2/C ratio gave variating results. With a ST/C ratio of 1.62 was the highest fraction of H2 in the outlet when the O2/C ratio was 0.53. The ratio highly affects the outlet temperature which again influence on the conversions and outlet compositions. It is seen in literature that the optimum ratio is affected by the inlet temperature, ST/C ratio and pressure, and should therefore be the last parameter to be optimized. It should also be mentioned that the equilibrium temperature increases with an increasing O2/C ratio. This is not evaluated further but in the range 0.5-0.6 should be adequate for this purpose.

- Low inlet temperature to the WGS reactors. As low as possible within the limits of the catalyst and the dew point of the inlet gas.
- The energy out of the burner (to the cracking furnace) is maximized when the inlet is combusted stoichiometrically.

With the points stated above in mind is there definitely sufficient amount of information to make the system be more efficient, convert enough, and to produce more hydrogen. But, as mentioned previously, is it close to impossible to design the most optimal system when the cost equation is out of the calculation. However, these results, findings, and results may be utilized in the further project steps and it gives information to conclude and answer the overall question "Is this a possibility? And what may be the next steps?".

When selecting a case for further development is the hydrogen feed to the burner a reasonable place to start, as this should be as high as possible and relates to the conversions in the reactors. Case 0 has a flow of 4450kmole/h and Case 4 has 4235kmole/h. There are some alterations to the process that will lead to a higher hydrogen production. For Case 4 is 4252kmole/h achieved when the inlet flow exactly meets vapor fraction of 1. Two reactors with the associated equipment, catalysts and flow can be reduced to one, but a single reactor will lead to increase is several of the process flow which all comes at a cost. Even if the use of a MT-WGS reactor can be advantageous for hydrogen production and for the investment and operational cost, is the desire of producing more hydrogen outweighing this. This will not be discussed further as it is out of scope of this project. But this is meant as an underlining of the possibility of utilizing a MT-WGS. All in all, is this resulting in the further development of Case 2, and only Case 2.

7.3 Maximizing hydrogen production in an ATR process with integrated pre-combustion CO2 capture (Case 5)

Case 5 har its starting point from Case 2 that was described in section 6.3. A snapshot of the Aspen HYSYS simulation is presented in Figure 7.1 (identical to Case 2). Since the CO2 separation and H2 purification is not decided and absorption with MDEA and PSA is considered as the state-of-the-art technology is the pressure not reduced further. The reduction would improve the production rate but since there is likely to be a pressure requirement down the process line is it kept the same. The ST/C ratio is increased to 2, which is the highest value within the normal operating condition of an ATR (between 1 and 2). The inlet temperature to the ATR is risen from 650 to 750°C, and not higher due to assumed material and corrosion restrictions. Lastly is a case study to find the optimal O2/C ratio for this system and the peak in hydrogen production is when the flow of O2 is 310kmole/h, which corresponds to a ratio of 0.52. Slightly lower than the one observed for Case 2 (0.53). It should be noted that the amount and the composition in the recycle steam changes when parameter changes, causing some small variations in the ratios. Next is the inlet temperature to the HT- and LT-WGS reactors are kept at the (normal) minimum of 300 and 175°C, respectively. It is not unlikely that these temperatures can be even lower in the near future, if the catalyst development continues. The hydrogen produced in this system amount to 4659kmole/h H2, exceeding the amount that in section 6.1 was stated as the minimum (4565kmole/h) if the same ethylene production rate were to be kept. When burned stoichiometrically is the energy supply to the cracker -7.615e+008kJ/h. This is above what is necessary and can be reduced by reducing the ethane feed again, if desired.
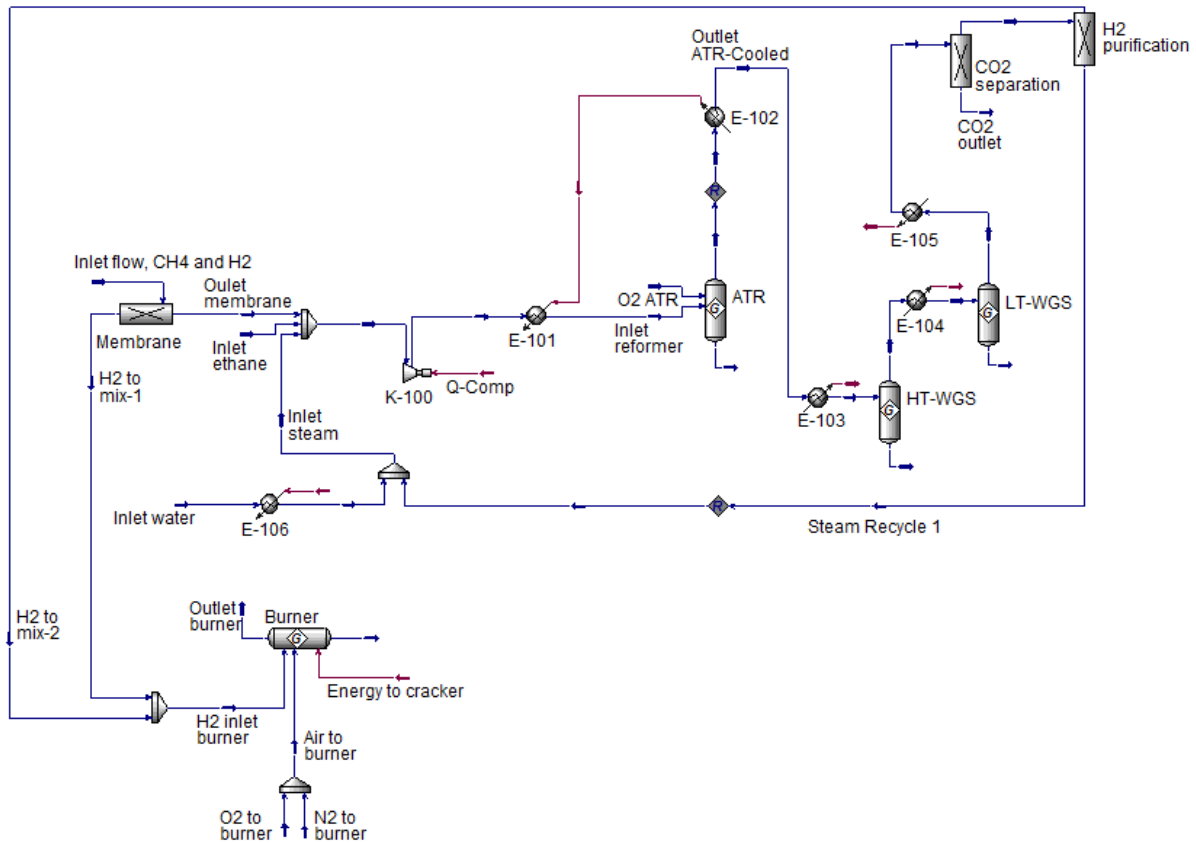
Figure 7.1 Snapshot from Aspen HYSYS of Case 5 (partly optimized)

If ethane is reduced to 22kmole/h (keeping temperature and ratios the same) will the hydrogen to the burner be 4571kmole/h. This is a sufficient amount and the energy from burner to the cracker will be -7.485e+008kJ/h.

Comparing Case 5 with Case 2 it can be seen that the recycle stream is increase (780.9 to 869.6kmole/h) and the H_2O molar composition is increased (0.64 to 0.67). This lowers to input of water to the system (804.4 to 573.1) but note that the ST/C ratio into the ATR remains the same. Another thing to take note of is the lowered flow in the CO_2 outlet (594.7 to 557.8). When comparing the outlet composition of the different substances can it also be seen that Case 5 has generally has higher fraction of CH_4 and H_2O and lower H_2, CO and CO_2. The energy flows were also higher which relates to the increase in flow throughout the system.

8 Pinch analysis for calculating possible steam analysis

This chapter presents a pinch analysis for Case 5. The first section includes the motivations for completing such analysis. The second section presents the approach to determine pinch temperatures and minimum utility loads. The third section presents a suggested design of a MER-network.

8.1 Motivation for pinch analysis

There are two major motivations for completing a pinch analysis of the process simulation. The first one is to determine if the system has a cooling or heating requirement (or both) and use the results to quantify how much that potentially must be imported or exported of steam or cooling. The second is to use the information for construct a MER-network. This method will, unlike the numbers found from Aspen HYSYS, lead to a minimum hot and cold utility which will be utilized in designing the MER-network. A question of interest that can be answered after such an analysis is "Is the simulated system self-supplied with thermal energy?" and "how much can potentially be exported?". This will provide useful information when designing the system. The method and approach are the same as presented in [67] and the minimum temperature difference is assumed to be 10°C.

8.2 Determine pinch temperatures and utilities for Case 5

The first step towards determining the pinch temperatures is to find the start (Ts) and target (Tt) temperatures for the involved streams. Second is to find or calculate the corresponding mass flow [kg/s] multiplied with the specific mass heat capacity [kJ/(kg*°C)]. The numbers are found from Aspen HYSYS, and the calculation results is presented in Table 8.1.

Table 8.1 Start and target temperatures with corresponding $\dot{m}Cp$ for Case 5

Stream	Type	Ts [°C]	Tt [°C]	$\dot{m}Cp$ [$kW/°C$]
C1 (Comp to ATR)	Cold	536.5	750.0	27.9
C2 (Inlet water to MIX)	Cold	15.0	99.96	12.5
H1 (ATR to HT-WGS)	Hot	948.0	300.0	32.0
H2 (HT-WGS to LT-WGS)	Hot	410.1	175.0	30.7
H3 (LT-WGS to CO2 separation)	Hot	211.7	200.0	30.3

The heat capacity for the various flow rates is assumed to be constant. This is a reasonable assumption since there are no changes is the phase of the flows, no reaction occurring, and the

temperature ranges are not too high. In addition is this a feasibility study, making the accuracy requirement lower. There is only one exception to this and that is the inlet water flow which evaporates in E-106 and in this case is the mCp for the liquid chosen. This is because the water barely reaches the evaporation limit (since its outlet temperature is just below 100°C at 1atm). This will not be completely accurate, but the result is evaluated as reasonable.

The second step is to calculate and list the modified temperatures from highest to lowest value. By this is it meant that 5°C is subtracted from the temperatures of the hot streams and 5 °C are added to the temperatures of the cold streams. The difference between two following temperatures in the list makes up the temperature interval (ΔT_{int}). The change in enthalpy (ΔH_{int}) is the value of the temperature interval is multiplied by "the sum of $\dot{m}Cp$ for the cold streams minus the sum of $\dot{m}Cp$ of the hot streams", as shown in equation (8.1).

$$\Delta H_{int} = \Delta T_{int} * \left(\sum \dot{m}Cp_c - \sum \dot{m}Cp_h \right) \qquad (8.1)$$

The summation of the ΔH for each interval multiplied with negative 1 will lead to the minimum hot utility load. This is the lowest value in the list for Case 5 is this 0 kW since there no negative values. The pinch temperature is the temperatures +/- 5°C around the temperature for the minimum hot utility load. In Case 5 was the hot pinch 948°C and the cold pinch 938°C. By making a starting point at zero and add the value of ΔH for each interval will the last interval be the minimum cold utility load. For Case 5 was the minimum cold utility load 21289.5kW. The minimum hot and cold utility load will be the target values in the MER-network design.

8.3 Design of MER-network for Case 5

The approach of the temperature interval method used. There are a few rules and guidelines that must complied with when designing the network. The $\dot{m}Cp$ rule states that above pinch must the $\dot{m}Cp, hot \leq \dot{m}Cp, cold$ and below pinch must $\dot{m}Cp, hot \geq \dot{m}Cp, cold$. The number of hot streams above pinch must equal or less than the cold streams and vis versa below pinch. In addition are cooling water not to be used above pinch and steam not to be used below pinch. Heat transfer across pinch is not allowed. The starting point is always at pinch temperature and the pinch exchangers and it is advantageous to maximize these duties first. So, having these points as the foundation can the MER-network presented in Figure 8.1 be the result. The arrows in the diagram states whether a stream is heated or cooled, and it is related to the tabulated values to the left in the figure. The $Qbelow$ is the $\dot{m}Cp$ multiplied with the temperature interval. As can be seen from the figure is there two process-to-process heat exchangers and three coolers. As stated in the previous section, the minimum hot utility is zero and this implies that there is only a need for a MER-network design below pinch. This can be verified from the network design. The cooling requirement (cold utility load) for the suggested network is the sum of the three coolers (Co 1, Co 2, and Co 3), which results in a cold utility load of 21287.7kW. This is less than 2kW higher than the minimum cold utility load that was determined in section 8.2. This can be explained by the use of constant Cp values or the number of digits used in calculations.

8 Pinch analysis for calculating possible steam analysis

Stream [-]	mCP [kW/°C]	Qbelow [kW]
H1	27.9	20727.0
H2	12.5	7215.1
H3	32	354.2
C1	30.7	5958.9
C2	30.3	1060.4
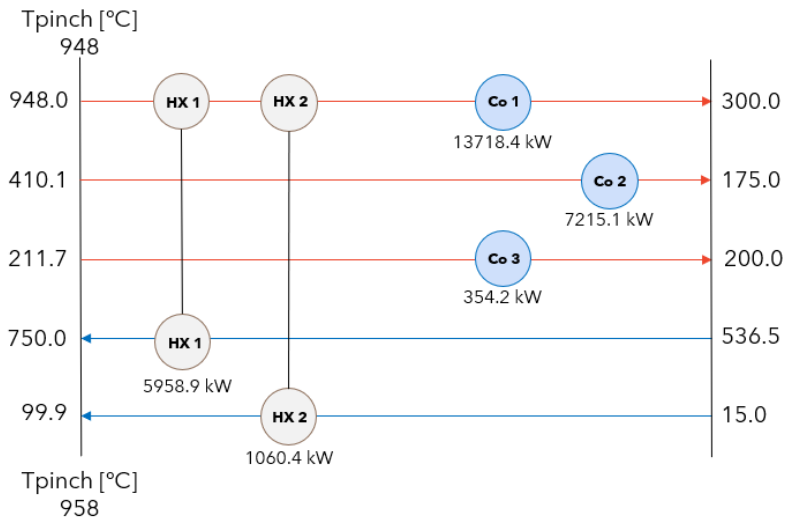
Figure 8.1 Suggested MER-network for Case 5

To verify that the number of heat exchangers is acceptable can the number of units be calculated as in equation (8.2). The result would be five heat exchangers, which matches the result.

$$Number\ of\ units\ =\ Number\ of\ streams\ -\ 1 \qquad (8.2)$$

As anticipated is there an excess of thermal energy, meaning that there is a possibility to export steam. At complex production plants, such as INEOS, where there is a heating requirement to numerous other parts of the process can this be a great advantage. The energy can be used both for pre-heating of the cracker inlet or to other parts of the system such as boilers. Alternatively, can the excess energy be utilized in the reforming system, for example pre-heating of the feed and air to the burner or other parts of the system. Since the technology for the CO2 and H2 separation is beyond the scope of this project could there also be use of the surplus energy in this section of the process. This is not discussed further in this section.

9 Evaluation and discussion

This chapter presents the evaluation and discussion for the work completed in this project. The first section includes the technology selection. The second section presents a general evaluation of the simulations in Aspen HYSYS. The third section evaluates the potential steam export before Case 5 is evaluated in the fourth section. The two last sections of this chapter, fifth and sixth, includes uncertainties and some suggestions for future work.

9.1 Tecnology selection

9.1.1 Selection of reforming technology

When faced with the descision of selecting the most suitable technology for this purpose was several aspects considered. Some of which was described in section 4.4. The most important might be that the hydrogen production should not have a massive carbon emission, due to the goal of reduction. This indicates that the reforming process should either have a low energy requirement or have the energy supplied from low-emitting source. In addition, the building of electrolyzers was close to the production site and added an interesting twist to the equation. Without further consideration the best suited reforming technology was chosen among those that utilized oxygen. This might not be the overall best choice when all asoects are considered. However, for the pupose of illustrating a possible option it is regarded as a good choice. After the ATR a traditional setup with two WGS reactors was chosen. An example of an innovative solution that could be considered is SE-WGS, as described in section 4.3.3.

The proposed flow sheet makes it possible to keep the existing plant layout of the cracking furnace, and only minor changes to the current process equipment can be expected. The exisiting equipment that are likely need most modifications or replacement is the burners. Another advantages is that the system is selfsupplied with thermal energy and there are no major piece of equipment that requires electrical energy except from the compressor. This is without considering the inlet membrane separation or the separation steps after the WGS reactors which will add to the energy accounts.

The reforming system itself includes implementation of several new process equipment. The cost evaluation is out of the scope for this project, but it should be underlined that he main economical question is how the cost of the reforming system compares to the cost of implementing a CO2 capture unit at every exhaust point. The suggested system is based on capturing CO2 pre-combustion, resulting in one capture point versus the twelve capure points necassary if the CO2 was capture at the furnace outlet.

If oxygen can be purchased at a reasonable price is another technology also of increased interest, namely the oxy-fuel combustion. The downside of this approach compared with pre-combustion capture is that the CO2 most be captured at several locations (all the furnaces). However, oxy-fuel combustion has not the need for implementation of large or costly process equipment, so there is a trade-off. Even if the oxy-fuel combustion is used without CO2 capture at the furnace outlet will the carbon emissions be reduced, as explained in section 3.3.2.

If there is no possibility to purchase oxygen at a low enough price (or not at all) and the ATR process still regarded as the most suitable technology, there is other alternatives. The oxygen

can be produced on site from air, for example by membrane. One interesting option called combined reforming and electrolysis (CRE) could also be considered. This is a configuration which combines the ATR with a water electrolysis. This way can the oxygen be produced on site and sent directly to the ATR, while the hydrogen can be sent directly to the cracker furnace as fuel. However, this system is not regarded as probable to be cost-competitive. Burning the hydrogen of such high quality might also considered to be a waste of resources. It could be more favorable to increase the production in the ATR so that the hydrogen produced in the electrolysis can be sold or utilized for other purposes. [62]

Last in this section will simulation of another reforming technology be shortly presented. The electric reformer was initially a option up for consideration because of its enormous potential to reduce emission and equipment size, as well as its improved efficiency and catalyst utilization. However, there are no electric reforming process for large scale production of hydrogen. The method requires more research as well as verifiction of the knowlegde from the lab-scale is valid at both pilot- and large-scale. It is simulated a base case that could represent the process of using an electric reformer. This simulation may be the starting point for others who wish to examine this option and is therefore included as Appendix E. The electric reformer can possibly be available within few years, keeping in mind that the first electric steam cracker is being designed and implemented in 2023. [38]

9.1.2 Selection of unit operations and configurations in Aspen HYSYS

The first process step is a separation unit for hydrogen and methane. By separating out the majority of the hydrogen prior to the reforming part is the flow throughout the system lowered, and along with it follows the cost. The separation unit can be a membrane with a selectivity of 95mol% for hydrogen. Other technologies could also be considered, for example adsorption. If the concept of using membrane is maintained must the specifications of the parameters (pressure, temperature, flows) and the membrane unit design be determined. Selection of this is out of the scope of the project.

All the configurations are described and evaluated in chapter 6. Other configurations that might be promising are using two reforming reactors. This can either be by installing a pre-reformer or by post-reformer. Installing a pre-reformer is traditionally installed when having higher hydrocarbon as feedstock but it might also improve conversion for lighter hydrocarbons. A post-reformer can be installation of an ATR after a SMR, but one can utilize CO_2 as well. [68]

All the simulated cases include a cooler after the last WGS reactor. This is cooling the stream to 200°C prior to the CO_2 separation unit. When the separation technology is decided might this change, perhaps can the cooler be excluded.

All simulated cases have CO_2 separation followed by H2 purification. The order is not absolute and may switch if proved to be more beneficial (both orders are found in literature). In this work is the order of the units regarded as equally good for the purpose of demonstrating a concept. As previously implied, a single separation unit (for example SE-WGS) can be utilized. The main challenge related to single unit operations is to achieve acceptable outlet purity for both the CO_2 and the H2, at a reasonable cost. However, most of the studies has purity requirements for the CO_2 and H2 leveling the ones for transport purposes. If the required purity can be lowered (for the H2), as mentioned previously, can one be curious if a single unit might

prove be the most attractive option. The selection of the separation technology is not discussed further.

9.2 General evaluation of simulations in Aspen HYSYS

9.2.1 Equation of state

All cases were simulated with Peng Robinson as the equation of state. This is a commonly applied package for gas processing of both hydrocarbons and hydrogen, and is suits for refinery and ethylene plants. [69] It is a fluid package which is capable of handling both hydrocarbons, air, water and combustion gases in the temperature and pressure scale relevant for this work [70]. A simulation of a similar system applied both Soave-Redlich-Kwong, Kabadi-Danner, and Peng-Robinson. Comparing the result revealed only minor. The relative difference in hydrogen production and natural gas input to the system that was approximately 0.02%. [62]

9.2.2 Choice of reactors

Normally is the ATR studied by minimizing the Gibbs free energy, such as the chosen reactor in Aspen HYSYS does. The downside of this approach for an ATR is that temperature and pressure is not constant in an adiabatic reactor. One reason is that the reactions occur sequentially (first the exothermic, then the endothermic). One alternative approach to do a thermodynamic analysis of such a system is to maximize the entropy of the system as performed by D. Souza [66]. This is not discussed further.

All the reactor used in the simulation are Gibbs reactors. There are five types of reactors that can be chosen in Aspen HYSYS; conversion, equilibrium, plug flow, continuous stirred flow, and Gibbs. The Gibbs reactor separates itself from the others by not requiring a set of reactions to be specified. In addition, the outlet properties do not have to be known/specified, at least when the reactor is simulated without an energy stream attached. If an energy stream is attached either the energy stream itself or the outlet temperature can be defined. The Gibbs reactor finds the equilibrium where the Gibbs free energy is at minimum. One should be aware that the calculation only includes the compositions specified in the component list. In the simulations presented in this work is that CH_4, C_2H_6, H_2, N_2, O_2, N_2, CO, CO_2, and H_2O.

There is variation in the literature of how the simulation of the ATR has been conducted. In [52] was the simulation of an ATR as a CSTR, PFR, and PFR as an adiabatic PFR (constant outlet temperature by adjusting O_2 flow) completed and compared with the goal of finding an optimal model for achieving a H_2/CO ratio around 2. It revealed that the ratio was (most likely) negatively affected by the WGS reactions and the complete combustion of CH_4, especially for the PFR. Overall did the work conclude that CSTR gave the best result among the three for producing syngas with the specific H_2/CO ratio from an ATR. Another study [62] simulated both an ATR and a furnace as Gibbs reactors but with the specifications of the equilibrium reactions. When comparing the molar fraction out of the ATR from that work and this work (Case 5) the results are similar (be aware that other operating conditions was not identical, and nitrogen is taken out of the equation). Presented here with a backslash (this work/that work) was molar compositions for CH_4 (0.0072/0.0032), H_2 (0.4704/0.4558), CO (0.1313/0.1693), CO_2 (0.0622/0.0609), and H_2O (0.3289/03108). In addition, the same work simulated the

WGS reactors as equilibrium reactors (and not Gibbs reactors). This was tested in this work, but the results between a Gibbs and an equilibrium reactor were identical. Overall, the choice of using Gibbs reactors for simulating the process is adequate at this stage, and the results are accurate enough for the purpose of demonstration.

9.2.3 Burner

Regarding the burner, there without doubt an error and it is idealized to a large extent. It is assumed that both fuels are burned stoichiometrically (maximizing heat output). This is not the case in reality where the stoichiometric fuel/air ratio is different from combusting hydrocarbons (0.05-0.07) then from combustion hydrogen (~0.03). In addition, the simulated energy flow from the burner representing the energy supply to the cracking furnace, has in reality a highly complex heat transfer system. The inclusion of this combustion reactor is only to illustrate that there is a possibility to cover the heat demand and use hydrogen as fuel to the furnace.

In retrospect there is one parameter to take special note of, namely the outlet temperature. The parameter was set to 850℃, being slightly above the outlet temperature of the cracking furnace. This temperature should have been increased because of the configuration of a furnace. The realistic temperature difference between the burner and the cracked gas inside the tubes, within the furnace, is much higher. A better suited temperature would be above 1000℃. One can argue how drastically this impact since the comparison between the burners are conducted with the same base. But it is definitely to be considered if utilizing the simulations in this work.

9.2.4 Contaminations

There is an assumption that the inlet process stream is without contaminations, like sulfur, salts, or other components. These contaminations could come from the cracking process or from the water (if there is a very strict requirement is the water demineralized). Either must the input already be so pure that no removal step is demanded, or purification step must be implemented. Alternatively, a leak can be included to prevent a potential buildup in the system (as some systems has) but this serves against the purpose of reducing emissions, if not sent back into the process somewhere. This is not discussed further.

9.2.5 Losses in the system

Pressure loss in the system is only considered for the heat exchangers and an assumed pressure loss in the separation processes that are simulated as component splitters. It is not included a pressure change over the reactors or in the pipes, and the assumed pressure drop in the heat exchangers could be higher than assumed. This should be more thoroughly evaluated if increased precision required. Especially, pressure loss over the reactors.

Other losses can be related to the process, both in regard to heat and to exergy. The heat losses are considered to be quite small compared to the exergy losses. In the suggested system (Case 5) is the exergy loss expected to be biggest in the transition between chemical and thermal energy (burner and ATR). Other exergy losses are in the heat exchangers, but those losses are assumed as minor. A. Behroozarand and D. A. Wood [71] calculated the exergy losses for different reformers used in hydrogen and syngas production. ATR showed the least loss in exergy when compared to the other configurations included in the study. The result was a loss

of 0.43 W per kilogram out of the reactor (on a dry basis). This included in this evaluation just to underline that there is a loss, and the aforementioned study can be a starting point if an exergy analysis of the system is desired. This is not discussed further.

9.2.6 Verification of the simulated system

To verify that the simulation and check if the main output are within a reasonable range, some simple calculations can be made. First, comparing the energy from the burner presented in section 6.1 with an industrial cracker producing ethylene. Assuming an annual ethylene production of approximate 650 000 ton with an energy demand to the cracker of 15GJ/ton ethylene (from [50]). As presented in equation (9.1) amounts this to 1219GJ/h, assuming 8000 operational hours per year.

$$\frac{650\,000\ \frac{ton}{year}}{8000\ \frac{h}{year}} * 15\,\frac{GJ}{ton} \approx 1219\,GJ/h \tag{9.1}$$

Comparing this with the output of Burner 2, which represents the fuel to the furnace, it can be seen that the numbers differ to some extent (7.5 to 12.2TJ/h). However, there are numerous unknowns and based on quite superficial and simple assumptions. Seeing that the numbers are in the same range is assumed to be adequate for its purpose. Another point to make is that the simulation of the two burners is made with equal operating conditions for both the H2 and the mix of H2 and CH4. Meaning that the energy from the burner of hydrogen must match the energy for the original mix. So, one can assume that ratio between the simulated and the 'real' cases can be acceptable.

A second verification is to confirm that the H2/CO-ratio of the simulated cases comply literature. The ratio is normally within the range of 3-5, out of a reformer [71]. The ratio for Case 0, Case 2, and Case 5 can be calculated from the outlet molar compositions of the ATR (available in Appendix B) and the result is 3.18, 3.05, and 3.58, respectively. All within the acceptable range.

9.3 Evaluation of Case 5

The simulation of Case 5 resulted in a higher H2 production than both Case 0 and Case 2, so to say that it has been partly optimized in this regard is correct. However, stating that it is absolutely maximized is not. Several measures can be made to enhance the production further. It may also be that the most optimal system produces less hydrogen if other factors are included. Some of the factors that might affect can be cracker configuration and reforming conditions such as pressure (dependent on downstream separation), reducing the flow in the recycle, other efficiencies than assumed, and of course the assumed ideality that brings deviation. Another factor is the temperatures in the system, such as the inlet temperature to the ATR. Mainly because high temperature correlates with extensive corrosion which leads to high material costs. This is why the upper limit is set to 750°C in this simulation (an assumed 'practical' limit which in reality can be lower or higher). In terms of methane conversion would an even higher inlet temperature be beneficial. When it comes to the ST/C ratio was is set to 2 which in some literature ([8]) was stated as the normal upper bound. Since the case revolved around

maximizing the hydrogen production would it favorable to increase this further, for example to 5 (as in [66]). However, it was kept within the most common range. The optimal O2/C ratio is regarded as a parameter with a little insecurity related to it. In Case 5 was it set to 0.52 which was the point that the hydrogen production peaked. As stated in the associated chapter is this a ratio where the optimum varies when other parameters are changed. The pressure is kept equal to the base case, but it should be minimized when the downstream process technologies has been selected. Literature agrees that a minimum pressure is most beneficial in regard to hydrogen yield but might be increased because of size and cost of the equipment.

What should be noted is that the recycle is not attached when conducting the case studies. This will bring a lowered accuracy. It is not attached due to converging calculations. Since the composition of the recycle is not pure water will the result deviate when compared to a simulation with an attached recycle. However, since this is a possibility study its regarded as acceptable. Natural next steps towards optimization could be the variation of more than 1 parameter at the time, including the cost equation. Since the main goal is reduction of carbon emissions, a natural parameter to minimize is the flow of CO2.

Increased flow of ethane is practical, but not necessarily the best nor most economical option. Figuring out what may be the best option for increased hydrogen production is not within the scope, but some alternatives are provided. Feeding more ethane to the steam cracker is one suggestion. This would result in a higher ethylene production and higher energy consumption. Moreover, the increase in hydrogen production would not necessarily outweigh the increased energy consumption to the cracker. A third option is to alter the cracking conditions so that more hydrogen and methane exits the cracker. For example, by a longer residence time. This would likely not cause an increase in energy, but it would likely result in less of the desired products. A fourth option is to purchase the hydrogen equal to the gap between actual and desired hydrogen flow to the burner. A fifth option is to feed other hydrocarbons into the reforming system that are more convenient or less costly. The best choice between the options will vary between the production sites and is not evaluated further.

The amount in the recycle is higher in Case 5 compared to Case 2. This relates to the slightly lower conversions of the methane and the slightly lower outlet temperature of the ATR. This might seem opposite of what is desired when maximizing the H2 production but the overall molar flow of H2 to the burner increases with these conditions. The amount in the recycle are highly affecting the equipment size because of its magnitude. This makes it reasonable to believe that the flow is lowered when the investment and operational cost are taken into consideration.

9.4 Potential steam export

A pinch analysis followed by a MER-network design gave a potential steam export of 21.3MW. What is important to underline is that some heat will be lost in the system and some heat might be required in the separation units (for example regeneration of ad/ab-sorbents). Additionally, the heat to the boilers is not considered in this work. The reasoning for this was that the complexity of a production plant such as INEOS, and its level of integrated heat/recovery systems, makes it hard to evaluate when the plant specifics is not known. It has also been regarded as less important than the steam cracker, making it second in line, and therefore fall outside of the scope for this work. It is reasonable to assume that a potential surplus of heat can

be utilized at existing plants such as INEOS. For example, to the boiler. It might also be beneficial of use the heat flow to increase the temperature of some of the involved streams in the reforming system, for example the inlet of air to the burner or the oxygen to the ATR. It was not a goal to maximize steam export, but it can definitely be an aspect of interest for further development of the system. Lastly, as mentioned previously, the utility loads and potential steam export will probably change after modifications are made. A final point is that it would be surprising if a surplus of energy from an ATR system located at a steam cracking plant (that has a high energy demand) would be lost, because of the many options for utilization.

9.5 Uncertainties

The process proposal comes with uncertainties and assumptions. I every uncertainty to every aspect, number, specification, assumption, process unit, and simplification were considered it would require a separate chapter. This is considered as unnecessary. This section provides the most obvious uncertainties so that it can add value to a potential evaluation for continuation of this work.

As presented in the chapter 4, there a lot of technologies to select from when it comes to reforming of hydrocarbons. Among the mature and well-tested technologies was the choice an ATR. One of the main motivations for this selection was the possibility of purchasing affordable oxygen. This assumption is based on the construction of water close to the INEOS production site. Normally, the oxygen production can make up over half the investment and operational cost of an ATR system. By eliminating this section and simply buy the oxygen, can the system be more favorable. However, this is only an assumption and brings uncertainty to the suggested system. Getting a price from the producers is a natural part of the next step to verify or reevaluate the system.

It is not considered the next step for the CO2 that has been captured. This adds uncertainty because it is not improbable that it has to be transported or shipped away. This is not considered of evaluated further but mentioned as an uncertainty. There are also uncertainties concerning the simulation. The uncertainties relate to the assumed ideality, the input parameters, the properties of the inlet flows, simplifications, and efficiencies. Several of these parameters are likely to be altered in a next step.

The last included uncertainty is an important one, namely the interest for reforming fuel to hydrogen as a decarbonization option in the industry. The industry is presented with a variety of options for reducing the carbon emissions, and it seems unlikely that every option is equally favored. Meaning that every industry and production plant that aims at lowering the emission are confronted with a decision. The uncertainty related to the decision would to a high degree affect which reduction option that receive most attention and resources for further development.

9.6 Future work

The continuation of this work can include several aspects and be completed by several approaches. This section will list some of the possibilities.
-   Obtaining plant specifics for evaluating possible integration, and verify or change assumed values in the simulation

- Design and evaluation of the separation units
- Quantify the CO2 reduction potential
- Inclusion of intermediate/buffer/storage/transport system of the included streams
- Investigate burner design
- Optimize the system with all unit operations included
- Economic analysis and cost evaluation
- Find potential oxygen price or determine what the oxygen price must be to make this an appealing option in a cost perspective
- LCA of the total system
- Comparing the price of this decarbonization option with other decarbonization options
- Map the interest in the industry

10 Conclusion

This work had four goals, all of which was achieved. A preparation for a literature review of the available decarbonization options for ethylene production by steam cracking has been presented. Showing that there are numerous methods to lower the carbon emissions associated with ethylene production. All the described methods has both advantages and disadvantages. Overall, one can say that process optimization, CCS, feedstock and/or fuel substitution appears to be most attractive when examining recent literature.

Regarding fuel substitution was reforming of the current fuel, consisting of both methane and hydrogen, to only hydrogen of particular interest. The suggested reforming process was an ATR process with integrated CO_2 capture prior the combustion. This system was simulated in Aspen HYSYS with five different configurations; Case 0 (base case), Case 1 (with recycle), Case 2 (adding ethane), Case 3 (Adding CO2), and Case 4 (MT-WGS). In addition, the effect of temperatures, pressure in reformer, ST/C-ratio, O2/C-ratio, excess O2 to burner and flow of CO_2 was analyzed and evaluated. These studies assisted in the evaluation and the results matched literature findings to a high degree. The information obtained was used to enhance the hydrogen production and simulate a system (Case 5) that was partly optimized to increase the hydrogen production.

Another goal was to investegate if reforming of methane to hydrogen is an applicable method to replace the current fuel, and thereby reducing the carbon emissions. The answer was no, the reforming of current fuel alone is not enough under the studied conditions. However, implementing a second inlet stream will result in a sufficient amount. The result was a system with a pressure of 2290kPa (in ATR), ST/C-ratio of 2, O2/C-ratio of 0.52, and an inlet temperature to the ATR, HT- and LT-WGS reactors of 750°C, 300°C, and 175°C, respectively. An inlet flow of 514.2kmole/h methane and 2976.3kmole/h hydrogen, where 95mol% of the hydrogen is separated prior to the reformation process. To cover the gap between the simulated and desired flow of hydrogen was an inlet flow of ethane added to the process. By adding 22kmole/h of ethane is a satisfactory production of hydrogen reached. Additionally, a potential steam export was found to be 21.3MW, excluding the heat required the separation unit(s). Nevertheless, it should be underlined that this process is dependent of some assumptions, as stated in the report.

The final goal was to complete an evaluation. The evaluation revealed that this is a system with potential and should definity be on the list of decabonization options to be considered in the future. It also showed that there are quite a few uncetainties and there is more work to be done, especially related to the assumed purchasable oxygen and optimization of the system in regards to both H2, CO2, and cost. A natural next step might be to include all the separation units in the simulation, determine efficiencies, quantify the potential CO2 reduction, and evaluate the economical aspect.

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Appendices

Appendix A - Task Description

Appendix B - Simulation of the cases (variating configuration)

Appendix C - Comparison of burners

Appendix D - Results of case studies (variating parameters)

Appendix E - Simulation of an electric reforming process

Appendix A - Task description

U/N University of
South-Eastern Norway
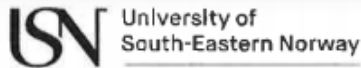
FMH606 Master's Thesis

Title: Reducing CO2 emissions of a gas cracker by reforming of fuel gas

USN supervisor: Klaus-Joachim Jens and Lars Erik Øi

External partners: INEOS Rafnes

Task background:
In order to reach international agreed climate targets current industry has to decarbonize emissions. The current project shall investigate decarbonization option(s) of a gas steam cracker exemplified by the INEOS Rafnes plant.

Task description:
The Rafnes steam cracker feedstock is ethane, which is converted to ethylene and some by-products. One by-product is fuel gas consisting of methane and hydrogen, which is used to heat cracking furnaces and boilers. Hence, there are several flue gas emission points to be scrubbed for CO2. Is it an alternative to reform fuel gas to pure hydrogen and use this hydrogen to heat furnaces and boilers? And what are the available reforming technologies to produce the hydrogen?

Work plan:
- Prepare a literature evaluation for reducing the CO2 emission related to ethylene production by steam cracking.
- Prepare a literature evaluation for reforming technologies
- Using preferably ASPEN-HYSYS software:
  - O Design and simulate a reforming process for the fuel gas to hydrogen that potentially can be used as fuel replacement to the ethane cracking furnace
  - O Evaluation of the suggested concept(s)

Student category: PT & EET

Practical arrangements: -

Supervision:
As a general rule, the student is entitled to 15-20 hours of supervision. This includes necessary time for the supervisor to prepare for supervision meetings (reading material to be discussed, etc.).

Signatures:

Supervisor (date and signature):

Student (capitalized letters): EMMY KRISTINE LINDELØFF RUSTAD

Student (date and signature):

Appendix B - Simulation of the cases (variating configurations)

Bold numbers refer to specified values and non-bold is calculated values. The stream names correspond with the snapshots of the flow sheets available in the report. Note that the energy to the heat exchangers (denoted as E-10X in table) can be cooling or heating demand.

Case 0

Stream properties			
Stream Name	Molar Flow [kmole/h]	Pressure [kPa]	Temperature [C]
Inlet flow. CH4 and H2	**3491**	**101.3**	**35**
Inlet water	835	111.3	**15**
Inlet steam	**835**	**101.3**	127.7
Inlet compressor	1498	101.3	84.33*
Outlet compressor	**1498**	**2300**	525.4
Inlet ATR	1498	2290	**650**
O2 ATR	**309**	**2290**	**25**
Outlet ATR	2519	2290	1050
Inlet HT-WGS	2519	2270	**300**
Outlet HT-WGS	2519	2270	421.8
Inlet LT-WGS	2519	2260	**175**
Outlet LT-WGS	2519	2260	220.3
Inlet CO2 separation	2519	2250	**200**
CO2 outlet	451.4	**2200**	202.5
Inlet H2 purification	2067	**2200**	**200**
Outlet H2 sep	617.9	**101.3**	191.2
H2 to mix-2	1449	**2000**	**200**
H2 to mix-1	2828	**101.3**	35.05
H2 inlet burner	4277	**101.3**	91.5
Outlet burner	12240	101.3	**850**
Air to burner	**10070**	**101.3**	**20**

*Vapour fraction = 1

Energy streams	
Equipment name	Energy [kJ/h]
K-100	2,66E+07
E-101	9,02E+06
E-102	9,02E+06
E-103	5,79E+07
E-104	2,10E+07
E-105	1,71E+06
E-106	4,05E+07
Energy from burner	-6,91E+08

Additional info	
EOS	PR
ST/C	1.62
O2/C	0.6

Molar compopsition							
Stream Name	CH4	H2	CO	CO2	H2O	O2	N2
Inlet flow. CH4 and H2	**0.1473**	**0.8527**	0	0	0	0	0
Inlet water	0	0	0	0	1	0	0
Inlet steam	0	0	0	0	1	0	0
Inlet compressor	0.3433	0.0993	0	0	0.5574	0	0
Outlet compressor	0.3433	0.0993	0	0	0.5574	0	0
Inlet ATR	0.3433	0.0993	0	0	0.5574	0	0
O2 ATR	0	0	0	0	0	1	0
Outlet ATR	0.0015	0.4749	0.1493	0.0533	0.321	0	0
Inlet HT-WGS	0.0015	0.4749	0.1493	0.0533	0.321	0	0
Outlet HT-WGS	0.0015	0.5818	0.0424	0.1602	0.214	0	0
Inlet LT-WGS	0.0015	0.5818	0.0424	0.1602	0.214	0	0
Outlet LT-WGS	0.0015	0.6198	0.0044	0.1982	0.176	0	0
Inlet CO2 separation	0.0015	0.6198	0.0044	0.1982	0.176	0	0
CO2 outlet	0	0.0035	0	0.9955	0.001	0	0
Inlet H2 purification	0.0019	0.7544	0.0053	0.0242	0.2142	0	0
Outlet H2 sep	0.0056	0.2524	0.0161	0.0808	0.6451	0	0
H2 to mix-2	0.0003	0.9684	0.0008	0	0.0306	0	0
H2 to mix-1	0	1	0	0	0	0	0
H2 inlet burner	0.0001	0.9893	0.0003	0	0.0104	0	0
Outlet burner	0	0.0002	0	0.0001	0.3493	0	0.6504
Air to burner	0	0	0	0	0	**0.21**	**0.79**

Case 1

Stream properties			
Stream Name	Molar Flow [kmole/h]	Pressure [kPa]	Temperature [C]
Inlet flow. CH4 and H2	**3491**	**101.3**	**35**
Inlet water	450.5	111.3	**15**
Inlet water heated	450.5	**101.3**	99.96
Inlet steam	**1093**	101.3	109.7
Inlet compressor	1756	101.3	80.35*
Outlet compressor	1756	**2300**	530.6
Inlet ATR	1756	2290	**650**
O2 ATR	**309**	2290	**25**
Outlet ATR	2783	2290	995.8
Inlet HT-WGS	2783	2270	**300**
Outlet HT-WGS	2783	2270	420.7
Inlet LT-WGS	2783	2260	**175**
Outlet LT-WGS	2783	2260	224.7
Inlet CO2 separation	2783	2250	**200**
CO2 outlet	514	**2200**	203.5
Inlet H2 purification	2269	**2200**	**200**
Steam Recycle	642.9	**101.3**	192.2
H2 to mix-2	1812	**2000**	**200**
H2 to mix-1	2828	**101.3**	35.05
H2 inlet burner	4453	**101.3**	95.83
Outlet burner	12740	101.3	**850**
Air to burner	**10490**	**101.3**	**20**

*Vapour fraction = 1

Energy streams	
Equipment name	Energy [kJ/h]
K-100	3,12E+07
E-101	9,77E+06
E-102	9,77E+06
E-103	5,85E+07
E-104	2,31E+07
E-105	2,29E+06
E-106	1,98E+07
Energy from burne	-7,20E+08

Additional info	
EOS	PR
ST/C	1.62
O2/C	0.6

Molar compopsition							
Stream Name	CH4	H2	CO	CO2	H2O	O2	N2
Inlet flow. CH4 and H2	**0.1473**	**0.8527**	0	0	0	0	0
Inlet water	0	0	0	0	**1**	0	0
Inlet steam	0	0	0	0	1	0	0
Inlet compressor	0.299	0.1847	0.0082	0.0324	0.4757	0	0
Outlet compressor	0.299	0.1847	0.0082	0.0324	0.4757	0	0
Inlet ATR	0.299	0.1847	0.0082	0.0324	0.4757	0	0
O2 ATR	0	0	0	0	0	1	0
Outlet ATR	0.0043	0.4843	0.153	0.057	0.3014	0	0
Inlet HT-WGS	0.0043	0.4843	0.153	0.057	0.3014	0	0
Outlet HT-WGS	0.0043	0.5901	0.0472	0.1628	0.1956	0	0
Inlet LT-WGS	0.0043	0.5901	0.0472	0.1628	0.1956	0	0
Outlet LT-WGS	0.0043	0.6316	0.0057	0.2043	0.1541	0	0
Inlet CO2 separation	0.0043	0.6316	0.0057	0.2043	0.1541	0	0
CO2 outlet	0	0.0034	0	0.9957	0.0008	0	0
Inlet H2 purification	0.0053	0.7739	0.007	0.0251	0.1888	0	0
Steam Recycle	0.0167	0.2731	0.0222	0.0884	0.5996	0	0
H2 to mix-2	0.0007	0.9719	0.001	0	0.0263	0	0
H2 to mix-1	0	1	0	0	0	0	0
H2 inlet burner	0.0003	0.9898	0.0004	0	0.0096	0	0
Outlet burner	0	0.0006	0	0.0002	0.3488	0	0.6504
Air to burner	0	0	0	0	0	**0.21**	**0.79**

Case 2

Stream properties			
Stream Name	Molar Flow [kmole/h]	Pressure [kPa]	Temperature [C]
Inlet flow. CH4 and H2	3491	101.3	35
Inlet water	804.4	111.3	15
Inlet water heated	804.4	101.3	99.96
Inlet steam	1303	101.3	111.2
Inlet ethane	40	101.3	35
Inlet compressor	2006	101.3	80.83*
Outlet compressor	2006	2300	525.6
Inlet ATR	2006	2290	650
O2 ATR	360	2290	25
Outlet ATR	3193	2290	1032
Inlet HT-WGS	3193	2270	300
Outlet HT-WGS	3193	2270	423.1
Inlet LT-WGS	3193	2260	175
Outlet LT-WGS	3193	2260	221.8
Inlet CO2 separation	3193	2250	200
CO2 outlet	594.7	2200	202.5
Inlet H2 purification	2599	2200	200
Steam Recycle	780.9	101.3	191.3
H2 to mix-2	1818	101.3	200
H2 to mix-1	2828	101.3	35.05
H2 inlet burner	4645	101.3	100.2
Outlet burner	13280	101.3	850
Air to burner	10920	101.3	20

*Vapour fraction = 1

Energy streams	
Equipment name	Energy [kJ/h]
K-100	3,56E+07
E-101	1,17E+07
E-102	1,17E+07
E-103	7,14E+07
E-104	2,69E+06
E-105	2,31E+06
E-106	2,30E+07
Energy from burner	-7,50E+08

Additional info	
EOS	PR
ST/C	1.62
O2/C	0.6

Molar compopsition							
Stream Name	CH4	C2H6	H2	CO	CO2	H2O	O2	N2
Inlet flow. CH4 and H2	0.1473	0	0.8527	0	0	0	0	0
Inlet water	0	0	0	0	0	1	0	0
Inlet steam	0	0	0	0	0	1	0	0
Inlet ethane	0	1	0	0	0	0	0	0
Inlet compressor	0.2592	0.0199	0.1717	0.0067	0.00328	0.5097	0	0
Outlet compressor	0.2592	0.0199	0.1717	0.0067	0.00328	0.5097	0	0
Inlet ATR	0.2592	0.0199	0.1717	0.0067	0.00328	0.5097	0	0
O2 ATR	0	0	0	0	0	0	1	0
Outlet ATR	0.002	0	0.4651	0.1526	0.0581	0.3222	0	0
Inlet HT-WGS	0.002	0	0.4651	0.1526	0.0581	0.3222	0	0
Outlet HT-WGS	0.002	0	0.5736	0.0441	0.1667	0.2137	0	0
Inlet LT-WGS	0.002	0	0.5736	0.0441	0.1667	0.2137	0	0
Outlet LT-WGS	0.002	0	0.613	0.0047	0.2061	0.1743	0	0
Inlet CO2 separation	0.002	0	0.613	0.0047	0.2061	0.1743	0	0
CO2 outlet	0	0	0.0033	0	0.9957	0.0009	0	0
Inlet H2 purification	0.0024	0	0.7525	0.0058	0.0253	0.214	0	0
Steam Recycle	0.0072	0	0.2507	0.0173	0.0844	0.6403	0	0
H2 to mix-2	0.0003	0	0.9682	0.0008	0	0.0306	0	0
H2 to mix-1	0	0	1	0	0	0	0	0
H2 inlet burner	0.0001	0	0.9876	0.0003	0	0.012	0	0
Outlet burner	0	0	0.0003	0	0.0002	0.3496	0	0.65
Air to burner	0		0	0	0	0	0.21	0.79

Case 3

Stream properties			
Stream Name	Molar Flow [kmole/h]	Pressure [kPa]	Temperature [C]
Inlet flow. CH4 and H:	3491	101.3	35
Inlet water	835	111.3	15
Inlet steam	835	101.3	127.7
Inlet compressor	1498	101.3	84.33*
Outlet compressor	1498	2300	525.4
Inlet ATR	1498	2290	650
O2 ATR	309	2290	25
CO2 ATR	75	2200	202.5
Outlet ATR	2268	2290	1050
Inlet HT-WGS	2268	2270	300
Outlet HT-WGS	2268	2270	435.1
Inlet LT-WGS	2268	2260	175
Outlet LT-WGS	2268	2260	249.4
Inlet CO2 separation	2519	2250	200
CO2 outlet	480.5	2200	203.8
Inlet H2 purification	1788	2200	200
Outlet H2 sep	406.2	101.3	195.6
H2 to mix-2	1381	2000	200
H2 to mix-1	2828	101.3	35.05
H2 inlet burner	4209	101.3	89.67
Outlet burner	12190	101.3	850
Air to burner	9968	101.3	20

*Vapour fraction = 1

Energy streams	
Equipment name	Energy [kJ/h]
K-100	2,05E+07
E-101	8,76E+06
E-102	8,76E+06
E-103	5,07E+07
E-104	1,98E+07
E-105	3,74E+06
E-106	2,52E+07
Energy from burner	-6,84E+08

Additional info	
EOS	PR
ST/C	1
O2/C	0.6

Molar compopsition							
Stream Name	CH4	H2	CO	CO2	H2O	O2	N2
Inlet flow. CH4 and H:	0.1473	0.8527	0	0	0	0	0
Inlet water	0	0	0	0	1	0	0
Inlet steam	0	0	0	0	1	0	0
Inlet compressor	0.4368	0.1264	0	0	0.4368	0	0
Outlet compressor	0.4368	0.1264	0	0	0.4368	0	0
Inlet ATR	0.4368	0.1264	0	0	0.4368	0	0
O2 ATR	0	0	0	0	0	1	0
CO2 ATR	0	0	0	1	0	0	0
Outlet ATR	0.0028	0.4871	0.2017	0.0553	0.2531	0	0
Inlet HT-WGS	0.0028	0.4871	0.2017	0.0553	0.2531	0	0
Outlet HT-WGS	0.0028	0.6044	0.0844	0.1726	0.1358	0	0
Inlet LT-WGS	0.0028	0.6044	0.0844	0.1726	0.1358	0	0
Outlet LT-WGS	0.0028	0.6664	0.0224	0.2345	0.0738	0	0
Inlet CO2 separation	0.0028	0.6664	0.0224	0.2345	0.0738	0	0
CO2 outlet	0	0.0031	0	0.9964	0.0003	0	0
Inlet H2 purification	0.0036	0.8447	0.0285	0.0298	0.0936	0	0
Outlet H2 sep	0.0141	0.3717	0.1127	0.131	0.3706	0	0
H2 to mix-2	0.0005	0.9838	0.0037	0	0.0121	0	0
H2 to mix-1	0	1	0	0	0	0	0
H2 inlet burner	0.0002	0.9947	0.0012	0	0.004	0	0
Outlet burner	0	0.0006	0	0.0005	0.3473	0	0.6516
Air to burner	0	0	0	0	0	0.21	0.79

Case 4

Stream properties			
Stream Name	Molar Flow [kmole/h]	Pressure [kPa]	Temperature [C]
Inlet flow. CH4 and H:	3491	101.3	35
Inlet water	835	111.3	15
Inlet steam	835	101.3	127.7
Inlet compressor	1498	101.3	84.33*
Outlet compressor	1498	2300	525.4
Inlet ATR	1498	2290	650
O2 ATR	309	2290	25
Outlet ATR	2519	2290	1050
Inlet MT-WGS	2519	2270	225
Outlet MT-WGS	2519	2270	366
Inlet CO2 separation	2519	2260	200
CO2 outlet	397.2	2200	202.2
Inlet H2 purification	2122	2200	200
Outlet H2 sep	714.3	101.3	190.7
H2 to mix-2	1407	2000	200
H2 to mix-1	2828	101.3	35.05
H2 inlet burner	4235	101.3	90.43
Outlet burner	12220	101.3	850
Air to burner	9945	101.3	20

*Vapour fraction = 1

Energy streams	
Equipment name	Energy [kJ/h]
K-100	2,66E+07
E-101	9,15E+06
E-102	9,15E+06
E-103	6,41E+07
E-104	1,42E+07
E-106	4,05E+07
Energy from burner	-6,82E+08

Additional info	
EOS	PR
ST/C	1.62
O2/C	0.6

Molar compopsition							
Stream Name	CH4	H2	CO	CO2	H2O	O2	N2
Inlet flow. CH4 and H:	0.1473	0.8527	0	0	0	0	0
Inlet water	0	0	0	0	1	0	0
Inlet steam	0	0	0	0	1	0	0
Inlet compressor	0.3433	0.0993	0	0	0.5574	0	0
Outlet compressor	0.3433	0.0993	0	0	0.5574	0	0
Inlet ATR	0.3433	0.0993	0	0	0.5574	0	0
O2 ATR	0	0	0	0	0	1	0
Outlet ATR	0.0015	0.4749	0.1493	0.0533	0.321	0	0
Inlet MT-WGS	0.0015	0.4749	0.1493	0.0533	0.321	0	0
Outlet MT-WGS	0.0015	0.5959	0.0283	0.1743	0.2	0	0
Inlet CO2 separation	0.0015	0.5959	0.0283	0.1743	0.2	0	0
CO2 outlet	0	0.0038	0.0002	0.9948	0.0013	0	0
Inlet H2 purification	0.0018	0.7067	0.0336	0.0207	0.2372	0	0
Outlet H2 sep	0.0049	0.2099	0.0898	0.0615	0.6339	0	0
H2 to mix-2	0.0003	0.9589	0.0051	0	0.0358	0	0
H2 to mix-1	0.0036	0.8447	0.0285	0.0298	0.0936	0	0
H2 inlet burner	0.0001	0.9863	0.0017	0	0.0119	0	0
Outlet burner	0	0.0007	0	0.0006	0.3489	0	0.6497
Air to burner	0	1	0	0	0	0.21	0.79

Case 5

Stream properties			
Stream Name	Molar Flow [kmole/h]	Pressure [kPa]	Temperature [C]
Inlet flow. CH4 and H2	**3491**	**101.3**	**35**
Inlet water	573.1	111.3	**15**
Inlet water heated	573.1	**101.3**	99.96
Inlet steam	**1442**	101.3	108.8
Inlet ethane	**22**	**101.3**	**35**
Inlet compressor	2127	101.3	83.69*
Outlet compressor	2127	**2300**	536.5
Inlet ATR	2127	2290	**650**
O2 ATR	**302.4**	2290	**25**
Outlet ATR	3239	2290	948
Inlet HT-WGS	3239	2270	**300**
Outlet HT-WGS	3239	2270	410.1
Inlet LT-WGS	3239	2260	**175**
Outlet LT-WGS	3239	2260	211.7
Inlet CO2 separation	3239	2250	**200**
CO2 outlet	557.8	**2200**	202.2
Inlet H2 purification	2681	**2200**	**200**
Steam Recycle	869.6	**101.3**	190.5
H2 to mix-2	1812	**101.3**	**200**
H2 to mix-1	2828	**101.3**	35.05
H2 inlet burner	4639	**101.3**	100.1
Outlet burner	13260	101.3	**850**
Air to burner	**10920**	**101.3**	**20**

*Vapour fraction = 1

Energy streams	
Equipment name	Energy [kJ/h]
K-100	3,80E+07
E-101	2,15E+07
E-102	2,15E+07
E-103	5,32E+07
E-104	2,59E+07
E-105	1,28E+06
E-106	2,51E+07
Energy from burner	-7,49E+07

Additional info	
EOS	PR
ST/C	2
O2/C	0.52

Molar compopsition							
Stream Name	CH4	C2H6	H2	CO	CO2	H2O	O2	N2
Inlet flow. CH4 and H2	**0.1473**	0	**0.8527**	0	0	0	0	0
Inlet water	0	0	0	0	0	1	0	0
Inlet steam	0	0	0	0	0	1	0	0
Inlet ethane	0	1	0	0	0	0	0	0
Inlet compressor	0.2517	0.0103	0.1611	0.0042	0.029	0.5437	0	0
Outlet compressor	0.2517	0.0103	0.1611	0.0042	0.029	0.5437	0	0
Inlet ATR	0.2517	0.0103	0.1611	0.0042	0.029	0.5437	0	0
O2 ATR	0	0	0	0	0	0	1	0
Outlet ATR	0.0072	0	0.4704	0.1313	0.0622	0.3289	0	0
Inlet HT-WGS	0.0072	0	0.4704	0.1313	0.0622	0.3289	0	0
Outlet HT-WGS	0.0072	0	0.5677	0.034	0.1595	0.2316	0	0
Inlet LT-WGS	0.0072	0	0.5677	0.034	0.1595	0.2316	0	0
Outlet LT-WGS	0.0072	0	0.5987	0.003	0.1904	0.2007	0	0
Inlet CO2 separation	0.0072	0	0.5987	0.003	0.1904	0.2007	0	0
CO2 outlet	0	0	0.0035	0	0.9953	0.0012	0	0
Inlet H2 purification	0.0087	0	0.7225	0.0036	0.023	0.2422	0	0
Steam Recycle	0.0244	0	0.2231	0.0102	0.071	0.6713	0	0
H2 to mix-2	0.0013	0	0.9623	0.0005	0	0.0358	0	0
H2 to mix-1	0	0	1	0	0	0	0	0
H2 inlet burner	0.0005	0	0.9853	0.0002	0	0.014	0	0
Outlet burner	0	0	0.0001	0	0.0002	0.3499	0	0.65
Air to burner	0	0	0	0	0	0	**0.21**	**0.79**

Appendix C - Comparison of burners

A snapshot of the Aspen HYSYS simulation is illustrated in Figure 6.1 and there is a description in the corresponding chapter. Burner 3 is a replica of Burner 1 with the exception of increased flows. The Burner 3 is used to illustrate the required amount of H2 to provide a sufficient amount of energy to the cracker. Note that the punctum (.) is replaces by comma (,) but has the same meaning as the punctum used previously. This is because the comma is more compatible with the Norwegian version of Excel.

Burner 1	Unit	H2	O2-1	N2-1	Air-1	Outlet-1	0-1	Q-1
Vapour Fraction		1,0	1,0	1,0	1,0	1,0	0,0	-
Temperature	C	100,0	20,0	20,0	20,0	850,0	850,0	-
Pressure	kPa	1000,0	101,3	101,3	101,3	101,3	101,3	-
Molar Flow	kgmole/h	4231,0	2115,5	7958,3	10073,8	12189,3	0,0	-
Mass Flow	kg/h	8529,7	67696,0	222936,1	290632,1	299158,0	0,0	-
Liquid Volume Flow	m3/h	122,1	59,5	276,5	336,0	352,8	0,0	-
Heat Flow	kJ/h	9061245,4	-329003,4	-1223014,2	-1552017,6	-685986865,5	0,0	-693496091,9

Burner 2	Unit	CH4+H2	O2-2	N2-2	Air-2	Outlet-2	0-2	Q-2
Vapour Fraction		1,0	1,0	1,0	1,0	1,0	0,0	-
Temperature	C	100,0	20,0	20,0	20,0	850,0	850,0	-
Pressure	kPa	1000,0	101,3	101,3	101,3	101,3	101,3	-
Molar Flow	kgmole/h	3491,0	2513,5	9455,6	11969,1	13975,3	0,0	-
Mass Flow	kg/h	14252,3	80432,6	264880,4	345313,0	359561,1	0,0	-
Liquid Volume Flow	m3/h	113,5	70,7	328,5	399,2	428,3	0,0	-
Heat Flow	kJ/h	-30721037,3	-390903,6	-1453117,8	-1844021,5	-780328005,9	0,0	-747762945,6

Burner 3	Unit	H2-3	O2-3	N2-3	Air-3	Outlet-3	0-3	Q-3
Vapour Fraction		1,0	1,0	1,0	1,0	1,0	0,0	-
Temperature	C	100,0	20,0	20,0	20,0	850,0	850,0	-
Pressure	kPa	1000,0	101,3	101,3	101,3	101,3	101,3	-
Molar Flow	kgmole/h	4565,0	2282,5	8586,5	10869,0	13151,6	0,0	-
Mass Flow	kg/h	9203,0	73040,0	240535,0	313575,0	322773,9	0,0	-
Liquid Volume Flow	m3/h	131,7	64,2	298,3	362,5	380,7	0,0	-
Heat Flow	kJ/h	9776550,5	-354975,3	-1319560,4	-1674535,7	-740139456,7	0,0	-748241470,0

Appendix D - Results of case studies (variating parameters)

Unless stated in the table is the following units valid; Temperature [°C], Molar Flow [kmole/h], Heat Flow [kJ/h], Pressure [kPa]. Note that the punctum (.) is replaces by comma (,) but has the same meaning as the punctum used previously. This is because the comma is more compatible with the Norwegian version of Excel. Another note is that that some of the tables exceeds one page, it will in such cases be continued at the following page.

Case study for ST/C-ratio

State	Outlet ATR-1 Temperature	Inlet stem Molar Flow	Q-102 Heat Flow	Outlet ATR-1 Master Comp Mole Flow (CO)	Outlet ATR-1 Master Comp Mole Flow (CO2)	Outlet ATR-1 Master Comp Mole Flow (H2O)	Outlet ATR-1 Master Comp Mole Flow (H2)	Outlet ATR-1 Master Comp Mole Flow (CH4)	Outlet ATR-1 Master Comp Mole Flow (O2)	Outlet ATR-1 Master Comp Mole Flow (Ethane)
Case 1	1214,3	300,0	1,03E+07	531,3	61,3	366,2	1227,7	1,7	0,00	0,00
Case 3	1204,3	340,0	1,03E+07	525,5	67,0	400,4	1233,5	1,7	0,00	0,00
Case 5	1194,8	380,0	1,03E+07	519,7	72,8	434,7	1239,2	1,7	0,00	0,00
Case 7	1185,6	420,0	1,04E+07	514,0	78,5	469,0	1244,8	1,7	0,00	0,00
Case 9	1176,9	460,0	1,04E+07	508,3	84,2	503,3	1250,5	1,7	0,00	0,00
Case 11	1168,5	500,0	1,04E+07	502,6	89,9	537,7	1256,0	1,8	0,00	0,00
Case 13	1160,5	540,0	1,04E+07	496,9	95,5	572,1	1261,6	1,8	0,00	0,00
Case 15	1152,7	580,0	1,05E+07	491,3	101,1	606,5	1267,1	1,8	0,00	0,00
Case 17	1145,3	620,0	1,05E+07	485,8	106,6	641,0	1272,5	1,9	0,00	0,00
Case 19	1138,1	660,0	1,05E+07	480,3	112,1	675,6	1277,9	1,9	0,00	0,00
Case 21	1131,2	700,0	1,06E+07	474,8	117,5	710,2	1283,2	1,9	0,00	0,00
Case 23	1124,5	740,0	1,06E+07	469,4	122,9	744,9	1288,5	2,0	0,00	0,00
Case 25	1118,1	780,0	1,06E+07	464,0	128,2	779,6	1293,7	2,0	0,00	0,00
Case 27	1111,8	820,0	1,07E+07	458,7	133,5	814,3	1298,9	2,0	0,00	0,00
Case 29	1105,8	860,0	1,07E+07	453,5	138,7	849,1	1304,0	2,1	0,00	0,00
Case 31	1099,9	900,0	1,08E+07	448,3	143,9	884,0	1309,0	2,1	0,00	0,00
Case 33	1094,3	940,0	1,08E+07	443,1	149,0	919,0	1314,0	2,1	0,00	0,00
Case 35	1088,8	980,0	1,09E+07	438,1	154,0	954,0	1319,0	2,2	0,00	0,00
Case 37	1083,4	1020,0	1,09E+07	433,0	159,0	989,0	1323,8	2,2	0,00	0,00
Case 39	1078,3	1060,0	1,09E+07	428,1	163,9	1024,1	1328,7	2,2	0,00	0,00
Case 41	1073,2	1100,0	1,10E+07	423,2	168,8	1059,3	1333,4	2,3	0,00	0,00
Case 43	1068,3	1140,0	1,10E+07	418,3	173,6	1094,5	1338,1	2,3	0,00	0,00
Case 45	1063,6	1180,0	1,11E+07	413,6	178,3	1129,8	1342,8	2,3	0,00	0,00
Case 47	1058,9	1220,0	1,11E+07	408,8	183,0	1165,2	1347,4	2,4	0,00	0,00
Case 49	1054,4	1260,0	1,12E+07	404,2	187,6	1200,6	1351,9	2,4	0,00	0,00
Case 51	1050,0	1300,0	1,12E+07	399,6	192,2	1236,0	1356,3	2,4	0,00	0,00
Case 53	1045,7	1340,0	1,13E+07	395,1	196,7	1271,6	1360,8	2,5	0,00	0,00
Case 55	1041,5	1380,0	1,13E+07	390,6	201,1	1307,1	1365,1	2,5	0,00	0,00
Case 57	1037,4	1420,0	1,14E+07	386,2	205,5	1342,8	1369,4	2,5	0,00	0,00
Case 59	1033,4	1460,0	1,14E+07	381,8	209,9	1378,5	1373,6	2,6	0,00	0,00
Case 61	1029,5	1500,0	1,15E+07	377,5	214,1	1414,3	1377,8	2,6	0,00	0,00
Case 63	1025,7	1540,0	1,15E+07	373,3	218,3	1450,1	1381,9	2,6	0,00	0,00
Case 65	1022,0	1580,0	1,16E+07	369,1	222,5	1485,9	1386,0	2,7	0,00	0,00
Case 67	1018,4	1620,0	1,16E+07	365,0	226,6	1521,9	1390,0	2,7	0,00	0,00
Case 69	1014,8	1660,0	1,17E+07	360,9	230,6	1557,9	1394,0	2,7	0,00	0,00
Case 71	1011,3	1700,0	1,17E+07	356,9	234,6	1593,9	1397,9	2,7	0,00	0,00
Case 73	1007,9	1740,0	1,18E+07	352,9	238,5	1630,0	1401,7	2,8	0,00	0,00
Case 75	1004,6	1780,0	1,18E+07	349,0	242,4	1666,1	1405,5	2,8	0,00	0,00
Case 77	1001,3	1820,0	1,19E+07	345,2	246,2	1702,3	1409,3	2,8	0,00	0,00
Case 79	998,1	1860,0	1,19E+07	341,4	250,0	1738,6	1413,0	2,8	0,00	0,00

Case 81	994,9	1900,0	1,20E+07	337,6	253,7	1774,9	1416,6	2,9	0,00	0,00
Case 83	991,8	1940,0	1,20E+07	333,9	257,4	1811,3	1420,2	2,9	0,00	0,00
Case 85	988,8	1980,0	1,21E+07	330,3	261,0	1847,7	1423,8	2,9	0,00	0,00
Case 87	985,9	2020,0	1,21E+07	326,7	264,6	1884,1	1427,3	2,9	0,00	0,00
Case 89	982,9	2060,0	1,22E+07	323,2	268,1	1920,6	1430,7	3,0	0,00	0,00
Case 91	980,1	2100,0	1,22E+07	319,7	271,5	1957,2	1434,1	3,0	0,00	0,00
Case 93	977,3	2140,0	1,23E+07	316,3	275,0	1993,8	1437,5	3,0	0,00	0,00
Case 95	974,5	2180,0	1,23E+07	312,9	278,3	2030,5	1440,8	3,0	0,00	0,00
Case 97	971,8	2220,0	1,24E+07	309,6	281,6	2067,2	1444,0	3,0	0,00	0,00
Case 99	969,2	2260,0	1,24E+07	306,3	284,9	2103,9	1447,2	3,1	0,00	0,00
Case 101	966,5	2300,0	1,25E+07	303,0	288,1	2140,7	1450,4	3,1	0,00	0,00
Case 103	964,0	2340,0	1,25E+07	299,8	291,3	2177,5	1453,5	3,1	0,00	0,00
Case 105	961,5	2380,0	1,26E+07	296,7	294,4	2214,4	1456,6	3,1	0,00	0,00
Case 107	959,0	2420,0	1,26E+07	293,6	297,5	2251,4	1459,7	3,1	0,00	0,00
Case 109	956,5	2460,0	1,27E+07	290,5	300,6	2288,3	1462,7	3,1	0,00	0,00
Case 111	954,1	2500,0	1,27E+07	287,5	303,6	2325,3	1465,6	3,2	0,00	0,00
Case 113	951,8	2540,0	1,28E+07	284,5	306,5	2362,4	1468,5	3,2	0,00	0,00
Case 115	949,4	2580,0	1,28E+07	281,6	309,5	2399,5	1471,4	3,2	0,00	0,00
Case 117	947,2	2620,0	1,29E+07	278,7	312,3	2436,6	1474,3	3,2	0,00	0,00
Case 119	944,9	2660,0	1,29E+07	275,8	315,2	2473,8	1477,1	3,2	0,00	0,00
Case 121	942,7	2700,0	1,30E+07	273,0	318,0	2511,0	1479,8	3,2	0,00	0,00
Case 123	940,5	2740,0	1,30E+07	270,3	320,7	2548,3	1482,6	3,2	0,00	0,00
Case 125	938,4	2780,0	1,31E+07	267,5	323,5	2585,6	1485,2	3,2	0,00	0,00
Case 127	936,2	2820,0	1,31E+07	264,8	326,1	2622,9	1487,9	3,3	0,00	0,00
Case 129	934,1	2860,0	1,32E+07	262,2	328,8	2660,3	1490,5	3,3	0,00	0,00
Case 131	932,1	2900,0	1,32E+07	259,6	331,4	2697,7	1493,1	3,3	0,00	0,00
Case 133	930,1	2940,0	1,33E+07	257,0	334,0	2735,1	1495,6	3,3	0,00	0,00
Case 135	928,1	2980,0	1,33E+07	254,4	336,5	2772,6	1498,1	3,3	0,00	0,00

Case study for O2/C-ratio

State	O2 ATR Molar Flow	Outlet ATR-1 Temperature	Outlet ATR-1 Molar Flow	Q-102 Heat Flow	Outlet ATR-1 Master Comp Mole Frac (CO)	Outlet ATR-1 Master Comp Mole Frac (CO2)	Outlet ATR-1 Master Comp Mole Frac (H2O)	Outlet ATR-1 Master Comp Mole Frac (H2)	Outlet ATR-1 Master Comp Mole Frac (CH4)	Outlet ATR-1 Master Comp Mole Frac (O2)	Outlet ATR-1 Master Comp Mole Frac (Ethane)
Case 1	120,0	725,0	2195,2	1,08E+07	0,0485	0,0700	0,3636	0,3657	0,1522	0,0000	0,0000
Case 2	125,0	730,2	2212,5	1,08E+07	0,0510	0,0704	0,3604	0,3710	0,1471	0,0000	0,0000
Case 3	130,0	735,3	2229,8	1,08E+07	0,0536	0,0708	0,3573	0,3762	0,1421	0,0000	0,0000
Case 4	135,0	740,4	2247,1	1,08E+07	0,0562	0,0711	0,3543	0,3813	0,1371	0,0000	0,0000
Case 5	140,0	745,3	2264,4	1,08E+07	0,0588	0,0714	0,3514	0,3862	0,1323	0,0000	0,0000
Case 6	145,0	750,3	2281,7	1,08E+07	0,0614	0,0716	0,3486	0,3910	0,1275	0,0000	0,0000
Case 7	150,0	755,1	2299,0	1,08E+07	0,0640	0,0717	0,3459	0,3957	0,1228	0,0000	0,0000
Case 8	155,0	759,9	2316,3	1,08E+07	0,0666	0,0718	0,3432	0,4002	0,1181	0,0000	0,0000
Case 9	160,0	764,7	2333,5	1,08E+07	0,0692	0,0719	0,3407	0,4047	0,1135	0,0000	0,0000
Case 10	165,0	769,5	2350,8	1,08E+07	0,0718	0,0719	0,3382	0,4090	0,1090	0,0000	0,0000
Case 11	170,0	774,2	2368,0	1,08E+07	0,0744	0,0719	0,3358	0,4132	0,1046	0,0000	0,0000
Case 12	175,0	778,9	2385,2	1,08E+07	0,0770	0,0719	0,3335	0,4173	0,1003	0,0000	0,0000
Case 13	180,0	783,5	2402,3	1,08E+07	0,0796	0,0718	0,3313	0,4214	0,0960	0,0000	0,0000
Case 14	185,0	788,2	2419,4	1,08E+07	0,0822	0,0717	0,3291	0,4253	0,0918	0,0000	0,0000
Case 15	190,0	792,9	2436,5	1,08E+07	0,0847	0,0716	0,3271	0,4290	0,0876	0,0000	0,0000
Case 16	195,0	797,5	2453,6	1,08E+07	0,0873	0,0714	0,3251	0,4327	0,0835	0,0000	0,0000
Case 17	200,0	802,2	2470,5	1,08E+07	0,0898	0,0712	0,3232	0,4363	0,0795	0,0000	0,0000
Case 18	205,0	806,9	2487,4	1,08E+07	0,0923	0,0710	0,3213	0,4398	0,0756	0,0000	0,0000
Case 19	210,0	811,6	2504,3	1,08E+07	0,0948	0,0707	0,3195	0,4432	0,0717	0,0000	0,0000
Case 20	215,0	816,4	2521,1	1,08E+07	0,0973	0,0705	0,3178	0,4465	0,0679	0,0000	0,0000
Case 21	220,0	821,2	2537,7	1,08E+07	0,0998	0,0702	0,3162	0,4496	0,0642	0,0000	0,0000
Case 22	225,0	826,1	2554,3	1,08E+07	0,1022	0,0699	0,3147	0,4527	0,0605	0,0000	0,0000
Case 23	230,0	831,0	2570,8	1,08E+07	0,1046	0,0696	0,3132	0,4556	0,0569	0,0000	0,0000
Case 24	235,0	836,0	2587,2	1,08E+07	0,1071	0,0692	0,3118	0,4585	0,0534	0,0000	0,0000
Case 25	240,0	841,1	2603,5	1,08E+07	0,1094	0,0689	0,3105	0,4612	0,0499	0,0000	0,0000
Case 26	245,0	846,4	2619,6	1,08E+07	0,1118	0,0685	0,3093	0,4638	0,0466	0,0000	0,0000
Case 27	250,0	851,7	2635,5	1,08E+07	0,1141	0,0681	0,3082	0,4663	0,0432	0,0000	0,0000
Case 28	255,0	857,2	2651,3	1,08E+07	0,1164	0,0677	0,3072	0,4687	0,0400	0,0000	0,0000
Case 29	260,0	862,9	2666,9	1,08E+07	0,1187	0,0672	0,3063	0,4709	0,0369	0,0000	0,0000
Case 30	265,0	868,8	2682,3	1,08E+07	0,1210	0,0668	0,3055	0,4730	0,0338	0,0000	0,0000
Case 31	270,0	874,9	2697,3	1,08E+07	0,1232	0,0663	0,3048	0,4749	0,0308	0,0000	0,0000
Case 32	275,0	881,2	2712,1	1,08E+07	0,1254	0,0658	0,3042	0,4767	0,0279	0,0000	0,0000
Case 33	280,0	887,9	2726,6	1,08E+07	0,1276	0,0652	0,3038	0,4783	0,0251	0,0000	0,0000
Case 34	285,0	894,9	2740,7	1,08E+07	0,1297	0,0647	0,3035	0,4797	0,0224	0,0000	0,0000
Case 35	290,0	902,3	2754,3	1,08E+07	0,1318	0,0641	0,3034	0,4808	0,0198	0,0000	0,0000
Case 36	295,0	910,3	2767,5	1,08E+07	0,1339	0,0635	0,3035	0,4818	0,0174	0,0000	0,0000
Case 37	300,0	918,7	2780,0	1,08E+07	0,1359	0,0629	0,3038	0,4824	0,0150	0,0000	0,0000
Case 38	305,0	927,9	2791,9	1,08E+07	0,1378	0,0622	0,3044	0,4828	0,0128	0,0000	0,0000
Case 39	310,0	937,7	2803,0	1,08E+07	0,1397	0,0615	0,3052	0,4828	0,0108	0,0000	0,0000
Case 40	315,0	948,4	2813,3	1,08E+07	0,1415	0,0608	0,3063	0,4824	0,0089	0,0000	0,0000

Case 41	320,0	960,1	2822,6	1,08E+07	0,1432	0,0600	0,3078	0,4817	0,0073	0,0000	0,0000
Case 42	325,0	972,8	2830,8	1,08E+07	0,1449	0,0593	0,3096	0,4805	0,0058	0,0000	0,0000
Case 43	330,0	986,5	2837,9	1,08E+07	0,1464	0,0584	0,3118	0,4788	0,0045	0,0000	0,0000
Case 44	335,0	1001,5	2843,8	1,08E+07	0,1479	0,0576	0,3143	0,4767	0,0035	0,0000	0,0000
Case 45	340,0	1017,5	2848,6	1,08E+07	0,1492	0,0568	0,3172	0,4742	0,0026	0,0000	0,0000
Case 46	345,0	1034,5	2852,4	1,08E+07	0,1505	0,0559	0,3204	0,4713	0,0019	0,0000	0,0000
Case 47	350,0	1052,3	2855,4	1,08E+07	0,1516	0,0551	0,3238	0,4681	0,0014	0,0000	0,0000
Case 48	355,0	1070,8	2857,5	1,08E+07	0,1526	0,0543	0,3274	0,4646	0,0010	0,0000	0,0000
Case 49	360,0	1089,9	2859,2	1,08E+07	0,1536	0,0535	0,3312	0,4610	0,0008	0,0000	0,0000
Case 50	365,0	1109,3	2860,3	1,08E+07	0,1544	0,0528	0,3351	0,4572	0,0006	0,0000	0,0000
Case 51	370,0	1129,0	2861,2	1,08E+07	0,1552	0,0521	0,3390	0,4533	0,0004	0,0000	0,0000
Case 52	375,0	1148,9	2861,8	1,08E+07	0,1559	0,0514	0,3429	0,4494	0,0003	0,0000	0,0000
Case 53	380,0	1168,9	2862,3	1,08E+07	0,1565	0,0508	0,3469	0,4455	0,0002	0,0000	0,0000
Case 54	385,0	1188,9	2862,6	1,08E+07	0,1571	0,0503	0,3508	0,4416	0,0002	0,0000	0,0000
Case 55	390,0	1209,0	2862,8	1,08E+07	0,1577	0,0498	0,3547	0,4377	0,0001	0,0000	0,0000
Case 56	395,0	1229,0	2863,0	1,08E+07	0,1581	0,0493	0,3587	0,4338	0,0001	0,0000	0,0000
Case 57	400,0	1249,0	2863,1	1,08E+07	0,1586	0,0489	0,3625	0,4299	0,0001	0,0000	0,0000
Case 58	405,0	1268,9	2863,2	1,08E+07	0,1590	0,0485	0,3664	0,4261	0,0001	0,0000	0,0000
Case 59	410,0	1288,8	2863,3	1,08E+07	0,1593	0,0482	0,3702	0,4223	0,0000	0,0000	0,0000
Case 60	415,0	1308,6	2863,3	1,08E+07	0,1596	0,0479	0,3740	0,4185	0,0000	0,0000	0,0000
Case 61	420,0	1328,3	2863,4	1,08E+07	0,1599	0,0476	0,3777	0,4147	0,0000	0,0000	0,0000
Case 62	425,0	1348,0	2863,4	1,08E+07	0,1602	0,0473	0,3815	0,4110	0,0000	0,0000	0,0000
Case 63	430,0	1367,5	2863,4	1,08E+07	0,1604	0,0471	0,3852	0,4073	0,0000	0,0000	0,0000
Case 64	435,0	1386,9	2863,4	1,08E+07	0,1606	0,0469	0,3888	0,4036	0,0000	0,0000	0,0000
Case 65	440,0	1406,2	2863,5	1,08E+07	0,1607	0,0468	0,3925	0,4000	0,0000	0,0000	0,0000
Case 66	445,0	1425,4	2863,5	1,08E+07	0,1609	0,0467	0,3961	0,3964	0,0000	0,0000	0,0000
Case 67	450,0	1444,5	2863,5	1,08E+07	0,1610	0,0466	0,3997	0,3928	0,0000	0,0000	0,0000
Case 68	455,0	1463,5	2863,5	1,08E+07	0,1610	0,0465	0,4032	0,3892	0,0000	0,0000	0,0000
Case 69	460,0	1482,3	2863,5	1,08E+07	0,1611	0,0464	0,4068	0,3857	0,0000	0,0000	0,0000
Case 70	465,0	1501,0	2863,5	1,08E+07	0,1611	0,0464	0,4103	0,3822	0,0000	0,0000	0,0000
Case 71	470,0	1519,6	2863,5	1,08E+07	0,1611	0,0464	0,4138	0,3787	0,0000	0,0000	0,0000
Case 72	475,0	1538,0	2863,5	1,08E+07	0,1611	0,0465	0,4172	0,3752	0,0000	0,0000	0,0000
Case 73	480,0	1556,3	2863,5	1,08E+07	0,1610	0,0465	0,4207	0,3718	0,0000	0,0000	0,0000
Case 74	485,0	1574,4	2863,5	1,08E+07	0,1610	0,0466	0,4241	0,3684	0,0000	0,0000	0,0000
Case 75	490,0	1592,4	2863,5	1,08E+07	0,1609	0,0466	0,4275	0,3650	0,0000	0,0000	0,0000
Case 76	495,0	1610,2	2863,5	1,08E+07	0,1608	0,0468	0,4309	0,3616	0,0000	0,0000	0,0000
Case 77	500,0	1627,9	2863,5	1,08E+07	0,1606	0,0469	0,4343	0,3582	0,0000	0,0000	0,0000
Case 78	505,0	1645,4	2863,5	1,08E+07	0,1605	0,0470	0,4376	0,3549	0,0000	0,0000	0,0000
Case 79	510,0	1662,7	2863,5	1,08E+07	0,1603	0,0472	0,4410	0,3515	0,0000	0,0000	0,0000
Case 80	515,0	1679,9	2863,5	1,08E+07	0,1602	0,0474	0,4443	0,3482	0,0000	0,0000	0,0000
Case 81	520,0	1696,9	2863,5	1,08E+07	0,1600	0,0476	0,4476	0,3449	0,0000	0,0000	0,0000
Case 82	525,0	1713,7	2863,5	1,08E+07	0,1598	0,0478	0,4508	0,3416	0,0000	0,0000	0,0000
Case 83	530,0	1730,3	2863,5	1,08E+07	0,1595	0,0480	0,4541	0,3384	0,0000	0,0000	0,0000
Case 84	535,0	1746,8	2863,5	1,08E+07	0,1593	0,0482	0,4574	0,3351	0,0000	0,0000	0,0000
Case 85	540,0	1763,0	2863,5	1,08E+07	0,1590	0,0485	0,4606	0,3319	0,0000	0,0000	0,0000
Case 86	545,0	1779,1	2863,5	1,08E+07	0,1588	0,0488	0,4638	0,3287	0,0000	0,0000	0,0000
Case 87	550,0	1795,0	2863,5	1,08E+07	0,1585	0,0491	0,4670	0,3255	0,0000	0,0000	0,0000
Case 88	555,0	1810,7	2863,5	1,08E+07	0,1582	0,0494	0,4702	0,3223	0,0000	0,0000	0,0000
Case 89	560,0	1826,2	2863,5	1,08E+07	0,1578	0,0497	0,4734	0,3191	0,0000	0,0000	0,0000
Case 90	565,0	1841,5	2863,5	1,08E+07	0,1575	0,0500	0,4765	0,3159	0,0000	0,0000	0,0000
Case 91	570,0	1856,7	2863,5	1,08E+07	0,1572	0,0504	0,4797	0,3128	0,0000	0,0000	0,0000
Case 92	575,0	1871,6	2863,5	1,08E+07	0,1568	0,0507	0,4828	0,3097	0,0000	0,0000	0,0000
Case 93	580,0	1886,3	2863,5	1,08E+07	0,1564	0,0511	0,4859	0,3065	0,0000	0,0000	0,0000
Case 94	585,0	1900,8	2863,5	1,08E+07	0,1560	0,0515	0,4890	0,3034	0,0000	0,0000	0,0000
Case 95	590,0	1915,2	2863,5	1,08E+07	0,1557	0,0519	0,4921	0,3003	0,0000	0,0000	0,0000
Case 96	595,0	1929,3	2863,5	1,08E+07	0,1552	0,0523	0,4952	0,2973	0,0000	0,0000	0,0000
Case 97	600,0	1943,2	2863,5	1,08E+07	0,1548	0,0527	0,4983	0,2942	0,0000	0,0000	0,0000

Case study: Pressure in ATR

State	Outlet ATR-1-2 Pressure	Outlet ATR-1 Temperature	Outlet ATR-1-2 Molar Flow	Outlet ATR-1-2 Master Comp Mole Frac (CO)	Outlet ATR-1-2 Master Comp Mole Frac (CO2)	Outlet ATR-1-2 Master Comp Mole Frac (Ethane)	Outlet ATR-1-2 Master Comp Mole Frac (H2O)	Outlet ATR-1-2 Master Comp Mole Frac (H2)	Outlet ATR-1-2 Master Comp Mole Frac (CH4)	Outlet ATR-1-2 Master Comp Mole Frac (N2)	Outlet ATR-1-2 Master Comp Mole Frac (O2)
Case 1	100,0	1088,1	2863,6	0,1540	0,0535	0,0000	0,3298	0,4627	0,0000	0,0000	0,0000
Case 2	200,0	1088,0	2863,5	0,1540	0,0535	0,0000	0,3298	0,4627	0,0000	0,0000	0,0000
Case 3	300,0	1087,9	2863,5	0,1540	0,0535	0,0000	0,3298	0,4626	0,0000	0,0000	0,0000
Case 4	400,0	1087,9	2863,4	0,1540	0,0535	0,0000	0,3298	0,4626	0,0000	0,0000	0,0000
Case 5	500,0	1087,8	2863,4	0,1540	0,0535	0,0000	0,3299	0,4626	0,0000	0,0000	0,0000
Case 6	600,0	1087,8	2863,3	0,1540	0,0535	0,0000	0,3299	0,4626	0,0001	0,0000	0,0000
Case 7	700,0	1087,8	2863,2	0,1539	0,0536	0,0000	0,3299	0,4625	0,0001	0,0000	0,0000
Case 8	800,0	1087,8	2863,0	0,1539	0,0536	0,0000	0,3300	0,4625	0,0001	0,0000	0,0000
Case 9	900,0	1087,8	2862,9	0,1539	0,0536	0,0000	0,3300	0,4624	0,0001	0,0000	0,0000
Case 10	1000,0	1087,9	2862,7	0,1539	0,0536	0,0000	0,3300	0,4624	0,0002	0,0000	0,0000
Case 11	1100,0	1087,9	2862,5	0,1539	0,0536	0,0000	0,3301	0,4623	0,0002	0,0000	0,0000
Case 12	1200,0	1088,0	2862,3	0,1539	0,0536	0,0000	0,3302	0,4622	0,0002	0,0000	0,0000
Case 13	1300,0	1088,1	2862,1	0,1538	0,0536	0,0000	0,3302	0,4621	0,0003	0,0000	0,0000
Case 14	1400,0	1088,2	2861,9	0,1538	0,0536	0,0000	0,3303	0,4620	0,0003	0,0000	0,0000
Case 15	1500,0	1088,3	2861,7	0,1538	0,0535	0,0000	0,3304	0,4619	0,0003	0,0000	0,0000
Case 16	1600,0	1088,4	2861,4	0,1538	0,0535	0,0000	0,3305	0,4618	0,0004	0,0000	0,0000
Case 17	1700,0	1088,6	2861,1	0,1537	0,0535	0,0000	0,3306	0,4617	0,0004	0,0000	0,0000
Case 18	1800,0	1088,8	2860,8	0,1537	0,0535	0,0000	0,3306	0,4616	0,0005	0,0000	0,0000
Case 19	1900,0	1088,9	2860,5	0,1537	0,0535	0,0000	0,3307	0,4615	0,0005	0,0000	0,0000
Case 20	2000,0	1089,1	2860,2	0,1537	0,0535	0,0000	0,3308	0,4614	0,0006	0,0000	0,0000
Case 21	2100,0	1089,3	2859,9	0,1536	0,0535	0,0000	0,3309	0,4612	0,0006	0,0000	0,0000
Case 22	2200,0	1089,6	2859,5	0,1536	0,0535	0,0000	0,3311	0,4611	0,0007	0,0000	0,0000
Case 23	2300,0	1089,8	2859,2	0,1536	0,0535	0,0000	0,3312	0,4610	0,0008	0,0000	0,0000
Case 24	2400,0	1090,0	2858,8	0,1535	0,0535	0,0000	0,3313	0,4608	0,0008	0,0000	0,0000
Case 25	2500,0	1090,3	2858,5	0,1535	0,0535	0,0000	0,3314	0,4607	0,0009	0,0000	0,0000
Case 26	2600,0	1090,6	2858,1	0,1535	0,0535	0,0000	0,3315	0,4605	0,0010	0,0000	0,0000
Case 27	2700,0	1090,8	2857,7	0,1534	0,0535	0,0000	0,3317	0,4604	0,0010	0,0000	0,0000
Case 28	2800,0	1091,1	2857,3	0,1534	0,0535	0,0000	0,3318	0,4602	0,0011	0,0000	0,0000
Case 29	2900,0	1091,4	2856,8	0,1534	0,0535	0,0000	0,3319	0,4600	0,0012	0,0000	0,0000
Case 30	3000,0	1091,7	2856,4	0,1533	0,0535	0,0000	0,3321	0,4599	0,0013	0,0000	0,0000
Case 31	3100,0	1092,1	2856,0	0,1533	0,0535	0,0000	0,3322	0,4597	0,0013	0,0000	0,0000
Case 32	3200,0	1092,4	2855,5	0,1533	0,0535	0,0000	0,3324	0,4595	0,0014	0,0000	0,0000
Case 33	3300,0	1092,7	2855,1	0,1532	0,0534	0,0000	0,3325	0,4593	0,0015	0,0000	0,0000
Case 34	3400,0	1093,1	2854,6	0,1532	0,0534	0,0000	0,3327	0,4591	0,0016	0,0000	0,0000

Case 35	3500,0	1093,4	2854,1	0,1531	0,0534	0,0000	0,3328	0,4589	0,0017	0,0000	0,0000
Case 36	3600,0	1093,8	2853,7	0,1531	0,0534	0,0000	0,3330	0,4588	0,0017	0,0000	0,0000
Case 37	3700,0	1094,1	2853,2	0,1531	0,0534	0,0000	0,3332	0,4586	0,0018	0,0000	0,0000
Case 38	3800,0	1094,5	2852,7	0,1530	0,0534	0,0000	0,3333	0,4584	0,0019	0,0000	0,0000
Case 39	3900,0	1094,9	2852,2	0,1530	0,0534	0,0000	0,3335	0,4582	0,0020	0,0000	0,0000
Case 40	4000,0	1095,3	2851,7	0,1529	0,0534	0,0000	0,3336	0,4580	0,0021	0,0000	0,0000
Case 41	4100,0	1095,7	2851,2	0,1529	0,0534	0,0000	0,3338	0,4578	0,0022	0,0000	0,0000
Case 42	4200,0	1096,0	2850,7	0,1529	0,0534	0,0000	0,3340	0,4575	0,0023	0,0000	0,0000
Case 43	4300,0	1096,4	2850,2	0,1528	0,0533	0,0000	0,3342	0,4573	0,0024	0,0000	0,0000
Case 44	4400,0	1096,8	2849,6	0,1528	0,0533	0,0000	0,3343	0,4571	0,0025	0,0000	0,0000
Case 45	4500,0	1097,3	2849,1	0,1527	0,0533	0,0000	0,3345	0,4569	0,0025	0,0000	0,0000
Case 46	4600,0	1097,7	2848,6	0,1527	0,0533	0,0000	0,3347	0,4567	0,0026	0,0000	0,0000
Case 47	4700,0	1098,1	2848,1	0,1526	0,0533	0,0000	0,3348	0,4565	0,0027	0,0000	0,0000
Case 48	4800,0	1098,5	2847,5	0,1526	0,0533	0,0000	0,3350	0,4563	0,0028	0,0000	0,0000
Case 49	4900,0	1098,9	2847,0	0,1526	0,0533	0,0000	0,3352	0,4561	0,0029	0,0000	0,0000
Case 50	5000,0	1099,3	2846,4	0,1525	0,0533	0,0000	0,3354	0,4558	0,0030	0,0000	0,0000
Case 51	5100,0	1099,8	2845,9	0,1525	0,0533	0,0000	0,3356	0,4556	0,0031	0,0000	0,0000
Case 52	5200,0	1100,2	2845,4	0,1524	0,0532	0,0000	0,3357	0,4554	0,0032	0,0000	0,0000
Case 53	5300,0	1100,6	2844,8	0,1524	0,0532	0,0000	0,3359	0,4552	0,0033	0,0000	0,0000
Case 54	5400,0	1101,1	2844,3	0,1523	0,0532	0,0000	0,3361	0,4549	0,0034	0,0000	0,0000
Case 55	5500,0	1101,5	2843,7	0,1523	0,0532	0,0000	0,3363	0,4547	0,0035	0,0000	0,0000
Case 56	5600,0	1101,9	2843,2	0,1522	0,0532	0,0000	0,3365	0,4545	0,0036	0,0000	0,0000
Case 57	5700,0	1102,4	2842,6	0,1522	0,0532	0,0000	0,3367	0,4543	0,0037	0,0000	0,0000
Case 58	5800,0	1102,8	2842,0	0,1521	0,0532	0,0000	0,3369	0,4540	0,0038	0,0000	0,0000
Case 59	5900,0	1103,2	2841,5	0,1521	0,0532	0,0000	0,3370	0,4538	0,0039	0,0000	0,0000
Case 60	6000,0	1103,7	2840,9	0,1520	0,0532	0,0000	0,3372	0,4536	0,0040	0,0000	0,0000
Case 61	6100,0	1104,1	2840,4	0,1520	0,0531	0,0000	0,3374	0,4534	0,0041	0,0000	0,0000
Case 62	6200,0	1104,6	2839,8	0,1520	0,0531	0,0000	0,3376	0,4531	0,0042	0,0000	0,0000
Case 63	6300,0	1105,0	2839,3	0,1519	0,0531	0,0000	0,3378	0,4529	0,0043	0,0000	0,0000
Case 64	6400,0	1105,5	2838,7	0,1519	0,0531	0,0000	0,3380	0,4527	0,0044	0,0000	0,0000
Case 65	6500,0	1105,9	2838,1	0,1518	0,0531	0,0000	0,3382	0,4524	0,0045	0,0000	0,0000
Case 66	6600,0	1106,4	2837,6	0,1518	0,0531	0,0000	0,3383	0,4522	0,0046	0,0000	0,0000
Case 67	6700,0	1106,8	2837,0	0,1517	0,0531	0,0000	0,3385	0,4520	0,0047	0,0000	0,0000
Case 68	6800,0	1107,3	2836,5	0,1517	0,0531	0,0000	0,3387	0,4518	0,0048	0,0000	0,0000
Case 69	6900,0	1107,7	2835,9	0,1516	0,0531	0,0000	0,3389	0,4515	0,0049	0,0000	0,0000
Case 70	7000,0	1108,1	2835,3	0,1516	0,0530	0,0000	0,3391	0,4513	0,0050	0,0000	0,0000
Case 71	7100,0	1108,6	2834,8	0,1515	0,0530	0,0000	0,3393	0,4511	0,0051	0,0000	0,0000
Case 72	7200,0	1109,0	2834,2	0,1515	0,0530	0,0000	0,3395	0,4508	0,0052	0,0000	0,0000
Case 73	7300,0	1109,5	2833,7	0,1514	0,0530	0,0000	0,3397	0,4506	0,0053	0,0000	0,0000
Case 74	7400,0	1109,9	2833,1	0,1514	0,0530	0,0000	0,3398	0,4504	0,0054	0,0000	0,0000
Case 75	7500,0	1110,4	2832,5	0,1513	0,0530	0,0000	0,3400	0,4502	0,0055	0,0000	0,0000
Case 76	7600,0	1110,8	2832,0	0,1513	0,0530	0,0000	0,3402	0,4499	0,0056	0,0000	0,0000
Case 77	7700,0	1111,3	2831,4	0,1512	0,0530	0,0000	0,3404	0,4497	0,0057	0,0000	0,0000
Case 78	7800,0	1111,7	2830,9	0,1512	0,0530	0,0000	0,3406	0,4495	0,0058	0,0000	0,0000
Case 79	7900,0	1112,1	2830,3	0,1512	0,0529	0,0000	0,3408	0,4493	0,0059	0,0000	0,0000
Case 80	8000,0	1112,6	2829,8	0,1511	0,0529	0,0000	0,3410	0,4490	0,0060	0,0000	0,0000
Case 81	8100,0	1113,0	2829,2	0,1511	0,0529	0,0000	0,3411	0,4488	0,0061	0,0000	0,0000
Case 82	8200,0	1113,5	2828,7	0,1510	0,0529	0,0000	0,3413	0,4486	0,0062	0,0000	0,0000
Case 83	8300,0	1113,9	2828,1	0,1510	0,0529	0,0000	0,3415	0,4483	0,0063	0,0000	0,0000
Case 84	8400,0	1114,3	2827,6	0,1509	0,0529	0,0000	0,3417	0,4481	0,0064	0,0000	0,0000
Case 85	8500,0	1114,8	2827,0	0,1509	0,0529	0,0000	0,3419	0,4479	0,0065	0,0000	0,0000
Case 86	8600,0	1115,2	2826,5	0,1508	0,0529	0,0000	0,3421	0,4477	0,0066	0,0000	0,0000
Case 87	8700,0	1115,6	2825,9	0,1508	0,0529	0,0000	0,3423	0,4474	0,0067	0,0000	0,0000
Case 88	8800,0	1116,1	2825,4	0,1507	0,0528	0,0000	0,3424	0,4472	0,0068	0,0000	0,0000
Case 89	8900,0	1116,5	2824,8	0,1507	0,0528	0,0000	0,3426	0,4470	0,0069	0,0000	0,0000
Case 90	9000,0	1116,9	2824,3	0,1506	0,0528	0,0000	0,3428	0,4468	0,0070	0,0000	0,0000
Case 91	9100,0	1117,4	2823,7	0,1506	0,0528	0,0000	0,3430	0,4466	0,0071	0,0000	0,0000
Case 92	9200,0	1117,8	2823,2	0,1505	0,0528	0,0000	0,3432	0,4463	0,0072	0,0000	0,0000
Case 93	9300,0	1118,2	2822,7	0,1505	0,0528	0,0000	0,3433	0,4461	0,0073	0,0000	0,0000
Case 94	9400,0	1118,7	2822,1	0,1505	0,0528	0,0000	0,3435	0,4459	0,0073	0,0000	0,0000
Case 95	9500,0	1119,1	2821,6	0,1504	0,0528	0,0000	0,3437	0,4457	0,0074	0,0000	0,0000
Case 96	9600,0	1119,5	2821,1	0,1504	0,0528	0,0000	0,3439	0,4455	0,0075	0,0000	0,0000
Case 97	9700,0	1119,9	2820,5	0,1503	0,0528	0,0000	0,3441	0,4452	0,0076	0,0000	0,0000
Case 98	9800,0	1120,4	2820,0	0,1503	0,0527	0,0000	0,3442	0,4450	0,0077	0,0000	0,0000
Case 99	9900,0	1120,8	2819,5	0,1502	0,0527	0,0000	0,3444	0,4448	0,0078	0,0000	0,0000
Case 100	10000.0	1121.2	2818.9	0.1502	0.0527	0.0000	0.3446	0.4446	0.0079	0.0000	0.0000

Case Study: Inlet temperature to HT-WGS

State	Inlet HT-WGS Temperature	Outlet HT-WGS Temperature	Outlet HT-WGS Molar Flow	Outlet HT-WGS Master Comp Mole Frac (CO)	Outlet HT-WGS Master Comp Mole Frac (CO2)	Outlet HT-WGS Master Comp Mole Frac (H2O)	Outlet HT-WGS Master Comp Mole Frac (H2)	Outlet HT-WGS Master Comp Mole Frac (CH4)	Outlet HT-WGS Master Comp Mole Frac (O2)	Outlet HT-WGS Master Comp Mole Frac (Ethane)
Case 1	250,0	388,5	2859,2	0,0334	0,1737	0,2110	0,5812	0,0008	0,0000	0,0000
Case 2	260,0	396,0	2859,2	0,0352	0,1718	0,2129	0,5793	0,0008	0,0000	0,0000
Case 3	270,0	403,4	2859,2	0,0371	0,1699	0,2148	0,5774	0,0008	0,0000	0,0000
Case 4	280,0	410,8	2859,2	0,0390	0,1680	0,2167	0,5755	0,0008	0,0000	0,0000
Case 5	290,0	418,2	2859,2	0,0410	0,1661	0,2186	0,5736	0,0008	0,0000	0,0000
Case 6	300,0	425,6	2859,2	0,0429	0,1642	0,2205	0,5716	0,0008	0,0000	0,0000
Case 7	310,0	433,0	2859,2	0,0449	0,1622	0,2225	0,5697	0,0008	0,0000	0,0000
Case 8	320,0	440,3	2859,2	0,0468	0,1603	0,2245	0,5677	0,0008	0,0000	0,0000
Case 9	330,0	447,7	2859,2	0,0488	0,1583	0,2264	0,5657	0,0008	0,0000	0,0000
Case 10	340,0	455,1	2859,2	0,0508	0,1563	0,2284	0,5638	0,0008	0,0000	0,0000
Case 11	350,0	462,6	2859,2	0,0527	0,1543	0,2304	0,5618	0,0008	0,0000	0,0000
Case 12	360,0	470,0	2859,2	0,0547	0,1523	0,2324	0,5598	0,0008	0,0000	0,0000
Case 13	370,0	477,4	2859,2	0,0567	0,1504	0,2343	0,5578	0,0008	0,0000	0,0000
Case 14	380,0	484,9	2859,2	0,0587	0,1484	0,2363	0,5559	0,0008	0,0000	0,0000
Case 15	390,0	492,3	2859,2	0,0607	0,1464	0,2383	0,5539	0,0008	0,0000	0,0000
Case 16	400,0	499,8	2859,2	0,0626	0,1444	0,2403	0,5519	0,0008	0,0000	0,0000
Case 17	410,0	507,3	2859,2	0,0646	0,1425	0,2422	0,5499	0,0008	0,0000	0,0000
Case 18	420,0	514,8	2859,2	0,0666	0,1405	0,2442	0,5480	0,0008	0,0000	0,0000
Case 19	430,0	522,4	2859,2	0,0685	0,1386	0,2461	0,5460	0,0008	0,0000	0,0000
Case 20	440,0	530,0	2859,2	0,0704	0,1366	0,2481	0,5441	0,0008	0,0000	0,0000
Case 21	450,0	537,6	2859,2	0,0724	0,1347	0,2500	0,5422	0,0008	0,0000	0,0000

Case Study: Inlet temperature to LT-WGS

State	Inlet LT-WGS Temperature	Outlet LT-WGS Temperature	Outlet LT-WGS Molar Flow	Outlet LT-WGS Master Comp Mole Frac (CO)	Outlet LT-WGS Master Comp Mole Frac (CO2)	Outlet LT-WGS Master Comp Mole Frac (H2O)	Outlet LT-WGS Master Comp Mole Frac (H2)	Outlet LT-WGS Master Comp Mole Frac (CH4)	Outlet LT-WGS Master Comp Mole Frac (O2)	Outlet LT-WGS Master Comp Mole Frac (Ethane)
Case 1	150,0	198,0	2859,2	0,0028	0,2043	0,1804	0,6118	0,0008	0,0000	0,0000
Case 2	155,0	202,6	2859,2	0,0031	0,2040	0,1807	0,6115	0,0008	0,0000	0,0000
Case 3	160,0	207,2	2859,2	0,0033	0,2037	0,1810	0,6112	0,0008	0,0000	0,0000
Case 4	165,0	211,8	2859,2	0,0037	0,2034	0,1813	0,6109	0,0008	0,0000	0,0000
Case 5	170,0	216,3	2859,2	0,0040	0,2031	0,1816	0,6106	0,0008	0,0000	0,0000
Case 6	175,0	220,8	2859,2	0,0043	0,2028	0,1820	0,6102	0,0008	0,0000	0,0000
Case 7	180,0	225,3	2859,2	0,0047	0,2024	0,1823	0,6098	0,0008	0,0000	0,0000
Case 8	185,0	229,8	2859,2	0,0051	0,2020	0,1827	0,6095	0,0008	0,0000	0,0000
Case 9	190,0	234,3	2859,2	0,0055	0,2016	0,1831	0,6090	0,0008	0,0000	0,0000
Case 10	195,0	238,7	2859,2	0,0059	0,2012	0,1835	0,6086	0,0008	0,0000	0,0000
Case 11	200,0	243,1	2859,2	0,0064	0,2007	0,1840	0,6082	0,0008	0,0000	0,0000
Case 12	205,0	247,5	2859,2	0,0068	0,2002	0,1845	0,6077	0,0008	0,0000	0,0000
Case 13	210,0	251,9	2859,2	0,0073	0,1998	0,1849	0,6072	0,0008	0,0000	0,0000
Case 14	215,0	256,2	2859,2	0,0078	0,1993	0,1855	0,6067	0,0008	0,0000	0,0000
Case 15	220,0	260,5	2859,2	0,0084	0,1987	0,1860	0,6062	0,0008	0,0000	0,0000
Case 16	225,0	264,8	2859,2	0,0089	0,1982	0,1865	0,6056	0,0008	0,0000	0,0000
Case 17	230,0	269,1	2859,2	0,0095	0,1976	0,1871	0,6051	0,0008	0,0000	0,0000
Case 18	235,0	273,3	2859,2	0,0101	0,1970	0,1877	0,6045	0,0008	0,0000	0,0000
Case 19	240,0	277,6	2859,2	0,0107	0,1964	0,1883	0,6039	0,0008	0,0000	0,0000
Case 20	245,0	281,8	2859,2	0,0113	0,1958	0,1889	0,6032	0,0008	0,0000	0,0000
Case 21	250,0	286,0	2859,2	0,0119	0,1951	0,1896	0,6026	0,0008	0,0000	0,0000

Case Study: Inlet temperature to MT-WGS

State	Inlet MT-WGS Temperature	Outlet MT-WGS Temperature	Outlet MT-WGS Molar Flow	Inlet MT-WGS Vapour Fraction	Outlet MT-WGS Master Comp Mole Frac (CH4)	Outlet MT-WGS Master Comp Mole Frac (H2)	Outlet MT-WGS Master Comp Mole Frac (ethane)	Outlet MT-WGS Master Comp Mole Frac (O2)	Outlet MT-WGS Master Comp Mole Frac (CO)	Outlet MT-WGS Master Comp Mole Frac (H2O)	Outlet MT-WGS Master Comp Mole Frac (CO2)
Case 1	150,0	185,3	2518,8	0,88	0,0015	0,6220	0,0000	0,0000	0,0022	0,1738	0,2004
Case 2	151,0	193,6	2518,8	0,88	0,0015	0,6216	0,0000	0,0000	0,0026	0,1742	0,2000
Case 3	152,0	202,0	2518,8	0,89	0,0015	0,6211	0,0000	0,0000	0,0031	0,1747	0,1995
Case 4	153,0	210,7	2518,8	0,90	0,0015	0,6205	0,0000	0,0000	0,0037	0,1753	0,1990
Case 5	154,0	219,5	2518,8	0,90	0,0015	0,6199	0,0000	0,0000	0,0043	0,1760	0,1983
Case 6	155,0	228,4	2518,8	0,91	0,0015	0,6191	0,0000	0,0000	0,0051	0,1767	0,1975
Case 7	156,0	237,6	2518,8	0,92	0,0015	0,6183	0,0000	0,0000	0,0059	0,1776	0,1967
Case 8	157,0	246,9	2518,8	0,93	0,0015	0,6173	0,0000	0,0000	0,0069	0,1786	0,1957
Case 9	158,0	256,4	2518,8	0,94	0,0015	0,6162	0,0000	0,0000	0,0080	0,1797	0,1946
Case 10	159,0	266,1	2518,8	0,95	0,0015	0,6149	0,0000	0,0000	0,0093	0,1809	0,1933
Case 11	160,0	276,0	2518,8	0,96	0,0015	0,6136	0,0000	0,0000	0,0107	0,1823	0,1920
Case 12	161,0	286,1	2518,8	0,97	0,0015	0,6120	0,0000	0,0000	0,0122	0,1838	0,1904
Case 13	162,0	296,4	2518,8	0,98	0,0015	0,6103	0,0000	0,0000	0,0139	0,1855	0,1887
Case 14	163,0	306,9	2518,8	0,99	0,0015	0,6085	0,0000	0,0000	0,0158	0,1874	0,1869
Case 15	164,0	317,6	2518,8	1,00	0,0015	0,6064	0,0000	0,0000	0,0178	0,1894	0,1848
Case 16	165,0	320,2	2518,8	1,00	0,0015	0,6059	0,0000	0,0000	0,0183	0,1899	0,1843
Case 17	166,0	321,0	2518,8	1,00	0,0015	0,6058	0,0000	0,0000	0,0184	0,1901	0,1842
Case 18	167,0	321,8	2518,8	1,00	0,0015	0,6056	0,0000	0,0000	0,0186	0,1902	0,1840
Case 19	168,0	322,5	2518,8	1,00	0,0015	0,6055	0,0000	0,0000	0,0188	0,1904	0,1839
Case 20	169,0	323,3	2518,8	1,00	0,0015	0,6053	0,0000	0,0000	0,0189	0,1905	0,1837
Case 21	170,0	324,1	2518,8	1,00	0,0015	0,6051	0,0000	0,0000	0,0191	0,1907	0,1836
Case 22	171,0	324,9	2518,8	1,00	0,0015	0,6050	0,0000	0,0000	0,0192	0,1909	0,1834
Case 23	172,0	325,7	2518,8	1,00	0,0015	0,6048	0,0000	0,0000	0,0194	0,1910	0,1832
Case 24	173,0	326,4	2518,8	1,00	0,0015	0,6047	0,0000	0,0000	0,0195	0,1912	0,1831
Case 25	174,0	327,2	2518,8	1,00	0,0015	0,6045	0,0000	0,0000	0,0197	0,1913	0,1829
Case 26	175,0	328,0	2518,8	1,00	0,0015	0,6044	0,0000	0,0000	0,0199	0,1915	0,1828
Case 27	176,0	328,7	2518,8	1,00	0,0015	0,6042	0,0000	0,0000	0,0200	0,1916	0,1826
Case 28	177,0	329,5	2518,8	1,00	0,0015	0,6040	0,0000	0,0000	0,0202	0,1918	0,1824
Case 29	178,0	330,3	2518,8	1,00	0,0015	0,6039	0,0000	0,0000	0,0203	0,1920	0,1823
Case 30	179,0	331,1	2518,8	1,00	0,0015	0,6037	0,0000	0,0000	0,0205	0,1921	0,1821
Case 31	180,0	331,8	2518,8	1,00	0,0015	0,6036	0,0000	0,0000	0,0207	0,1923	0,1820
Case 32	181,0	332,6	2518,8	1,00	0,0015	0,6034	0,0000	0,0000	0,0208	0,1924	0,1818
Case 33	182,0	333,4	2518,8	1,00	0,0015	0,6032	0,0000	0,0000	0,0210	0,1926	0,1816
Case 34	183,0	334,1	2518,8	1,00	0,0015	0,6031	0,0000	0,0000	0,0211	0,1928	0,1815
Case 35	184,0	334,9	2518,8	1,00	0,0015	0,6029	0,0000	0,0000	0,0213	0,1929	0,1813
Case 36	185,0	335,7	2518,8	1,00	0,0015	0,6027	0,0000	0,0000	0,0215	0,1931	0,1812
Case 37	186,0	336,5	2518,8	1,00	0,0015	0,6026	0,0000	0,0000	0,0216	0,1933	0,1810
Case 38	187,0	337,2	2518,8	1,00	0,0015	0,6024	0,0000	0,0000	0,0218	0,1934	0,1808
Case 39	188,0	338,0	2518,8	1,00	0,0015	0,6023	0,0000	0,0000	0,0220	0,1936	0,1807
Case 40	189,0	338,8	2518,8	1,00	0,0015	0,6021	0,0000	0,0000	0,0221	0,1938	0,1805

Case 41	190,0	339,5	2518,8	1,00	0,0015	0,6019	0,0000	0,0000	0,0223	0,1939	0,1803
Case 42	191,0	340,3	2518,8	1,00	0,0015	0,6018	0,0000	0,0000	0,0225	0,1941	0,1802
Case 43	192,0	341,0	2518,8	1,00	0,0015	0,6016	0,0000	0,0000	0,0226	0,1943	0,1800
Case 44	193,0	341,8	2518,8	1,00	0,0015	0,6014	0,0000	0,0000	0,0228	0,1944	0,1798
Case 45	194,0	342,6	2518,8	1,00	0,0015	0,6013	0,0000	0,0000	0,0230	0,1946	0,1797
Case 46	195,0	343,3	2518,8	1,00	0,0015	0,6011	0,0000	0,0000	0,0231	0,1948	0,1795
Case 47	196,0	344,1	2518,8	1,00	0,0015	0,6009	0,0000	0,0000	0,0233	0,1949	0,1793
Case 48	197,0	344,9	2518,8	1,00	0,0015	0,6008	0,0000	0,0000	0,0235	0,1951	0,1792
Case 49	198,0	345,6	2518,8	1,00	0,0015	0,6006	0,0000	0,0000	0,0236	0,1953	0,1790
Case 50	199,0	346,4	2518,8	1,00	0,0015	0,6004	0,0000	0,0000	0,0238	0,1954	0,1788
Case 51	200,0	347,1	2518,8	1,00	0,0015	0,6002	0,0000	0,0000	0,0240	0,1956	0,1787
Case 52	201,0	347,9	2518,8	1,00	0,0015	0,6001	0,0000	0,0000	0,0241	0,1958	0,1785
Case 53	202,0	348,7	2518,8	1,00	0,0015	0,5999	0,0000	0,0000	0,0243	0,1959	0,1783
Case 54	203,0	349,4	2518,8	1,00	0,0015	0,5997	0,0000	0,0000	0,0245	0,1961	0,1781
Case 55	204,0	350,2	2518,8	1,00	0,0015	0,5996	0,0000	0,0000	0,0246	0,1963	0,1780
Case 56	205,0	350,9	2518,8	1,00	0,0015	0,5994	0,0000	0,0000	0,0248	0,1964	0,1778
Case 57	206,0	351,7	2518,8	1,00	0,0015	0,5992	0,0000	0,0000	0,0250	0,1966	0,1776
Case 58	207,0	352,5	2518,8	1,00	0,0015	0,5990	0,0000	0,0000	0,0252	0,1968	0,1775
Case 59	208,0	353,2	2518,8	1,00	0,0015	0,5989	0,0000	0,0000	0,0253	0,1970	0,1773
Case 60	209,0	354,0	2518,8	1,00	0,0015	0,5987	0,0000	0,0000	0,0255	0,1971	0,1771
Case 61	210,0	354,7	2518,8	1,00	0,0015	0,5985	0,0000	0,0000	0,0257	0,1973	0,1769
Case 62	211,0	355,5	2518,8	1,00	0,0015	0,5984	0,0000	0,0000	0,0259	0,1975	0,1768
Case 63	212,0	356,3	2518,8	1,00	0,0015	0,5982	0,0000	0,0000	0,0260	0,1977	0,1766
Case 64	213,0	357,0	2518,8	1,00	0,0015	0,5980	0,0000	0,0000	0,0262	0,1978	0,1764
Case 65	214,0	357,8	2518,8	1,00	0,0015	0,5978	0,0000	0,0000	0,0264	0,1980	0,1762
Case 66	215,0	358,5	2518,8	1,00	0,0015	0,5977	0,0000	0,0000	0,0266	0,1982	0,1761
Case 67	216,0	359,3	2518,8	1,00	0,0015	0,5975	0,0000	0,0000	0,0267	0,1984	0,1759
Case 68	217,0	360,0	2518,8	1,00	0,0015	0,5973	0,0000	0,0000	0,0269	0,1985	0,1757
Case 69	218,0	360,8	2518,8	1,00	0,0015	0,5971	0,0000	0,0000	0,0271	0,1987	0,1755
Case 70	219,0	361,5	2518,8	1,00	0,0015	0,5970	0,0000	0,0000	0,0273	0,1989	0,1754
Case 71	220,0	362,3	2518,8	1,00	0,0015	0,5968	0,0000	0,0000	0,0274	0,1991	0,1752
Case 72	221,0	363,0	2518,8	1,00	0,0015	0,5966	0,0000	0,0000	0,0276	0,1992	0,1750
Case 73	222,0	363,8	2518,8	1,00	0,0015	0,5964	0,0000	0,0000	0,0278	0,1994	0,1748
Case 74	223,0	364,5	2518,8	1,00	0,0015	0,5962	0,0000	0,0000	0,0280	0,1996	0,1747
Case 75	224,0	365,3	2518,8	1,00	0,0015	0,5961	0,0000	0,0000	0,0281	0,1998	0,1745
Case 76	225,0	366,0	2518,8	1,00	0,0015	0,5959	0,0000	0,0000	0,0283	0,2000	0,1743
Case 77	226,0	366,8	2518,8	1,00	0,0015	0,5957	0,0000	0,0000	0,0285	0,2001	0,1741
Case 78	227,0	367,6	2518,8	1,00	0,0015	0,5955	0,0000	0,0000	0,0287	0,2003	0,1739
Case 79	228,0	368,3	2518,8	1,00	0,0015	0,5953	0,0000	0,0000	0,0289	0,2005	0,1738
Case 80	229,0	369,1	2518,8	1,00	0,0015	0,5952	0,0000	0,0000	0,0290	0,2007	0,1736
Case 81	230,0	369,8	2518,8	1,00	0,0015	0,5950	0,0000	0,0000	0,0292	0,2009	0,1734
Case 82	231,0	370,6	2518,8	1,00	0,0015	0,5948	0,0000	0,0000	0,0294	0,2010	0,1732
Case 83	232,0	371,3	2518,8	1,00	0,0015	0,5946	0,0000	0,0000	0,0296	0,2012	0,1730
Case 84	233,0	372,1	2518,8	1,00	0,0015	0,5944	0,0000	0,0000	0,0298	0,2014	0,1729
Case 85	234,0	372,8	2518,8	1,00	0,0015	0,5943	0,0000	0,0000	0,0299	0,2016	0,1727
Case 86	235,0	373,6	2518,8	1,00	0,0015	0,5941	0,0000	0,0000	0,0301	0,2018	0,1725
Case 87	236,0	374,3	2518,8	1,00	0,0015	0,5939	0,0000	0,0000	0,0303	0,2019	0,1723
Case 88	237,0	375,0	2518,8	1,00	0,0015	0,5937	0,0000	0,0000	0,0305	0,2021	0,1721
Case 89	238,0	375,8	2518,8	1,00	0,0015	0,5935	0,0000	0,0000	0,0307	0,2023	0,1720
Case 90	239,0	376,5	2518,8	1,00	0,0015	0,5934	0,0000	0,0000	0,0309	0,2025	0,1718
Case 91	240,0	377,3	2518,8	1,00	0,0015	0,5932	0,0000	0,0000	0,0310	0,2027	0,1716
Case 92	241,0	378,0	2518,8	1,00	0,0015	0,5930	0,0000	0,0000	0,0312	0,2028	0,1714
Case 93	242,0	378,8	2518,8	1,00	0,0015	0,5928	0,0000	0,0000	0,0314	0,2030	0,1712
Case 94	243,0	379,5	2518,8	1,00	0,0015	0,5926	0,0000	0,0000	0,0316	0,2032	0,1710
Case 95	244,0	380,3	2518,8	1,00	0,0015	0,5924	0,0000	0,0000	0,0318	0,2034	0,1709
Case 96	245,0	381,0	2518,8	1,00	0,0015	0,5923	0,0000	0,0000	0,0320	0,2036	0,1707
Case 97	246,0	381,8	2518,8	1,00	0,0015	0,5921	0,0000	0,0000	0,0321	0,2038	0,1705
Case 98	247,0	382,5	2518,8	1,00	0,0015	0,5919	0,0000	0,0000	0,0323	0,2040	0,1703
Case 99	248,0	383,3	2518,8	1,00	0,0015	0,5917	0,0000	0,0000	0,0325	0,2041	0,1701
Case 100	249,0	384,0	2518,8	1,00	0,0015	0,5915	0,0000	0,0000	0,0327	0,2043	0,1699
Case 101	250,0	384,8	2518,8	1,00	0,0015	0,5913	0,0000	0,0000	0,0329	0,2045	0,1697

Case Study: CO2 to ATR

State	CO2 ATR Molar Flow	Outlet ATR-1 Temperature	Outlet ATR-1 Molar Flow	Q-102 Heat Flow	Outlet ATR-1 Master Comp Mole Frac (CO)	Outlet ATR-1 Master Comp Mole Frac (CO2)	Outlet ATR-1 Master Comp Mole Frac (H2O)	Outlet ATR-1 Master Comp Mole Frac (H2)	Outlet ATR-1 Master Comp Mole Frac (CH4)	Outlet ATR-1 Master Comp Mole Frac (O2)	Outlet ATR-1 Master Comp Mole Frac (Ethane)
Case 1	0,0	1100,5	2198,6	8,73E+06	0,1907	0,0416	0,2411	0,5250	0,0016	0,0000	0,0000
Case 2	5,0	1096,9	2203,3	8,73E+06	0,1915	0,0424	0,2420	0,5223	0,0017	0,0000	0,0000
Case 3	10,0	1093,3	2207,9	8,73E+06	0,1924	0,0433	0,2429	0,5197	0,0018	0,0000	0,0000
Case 4	15,0	1089,8	2212,6	8,73E+06	0,1932	0,0442	0,2437	0,5171	0,0018	0,0000	0,0000
Case 5	20,0	1086,3	2217,3	8,73E+06	0,1940	0,0451	0,2446	0,5145	0,0019	0,0000	0,0000
Case 6	25,0	1082,8	2221,9	8,73E+06	0,1947	0,0460	0,2454	0,5119	0,0020	0,0000	0,0000
Case 7	30,0	1079,4	2226,6	8,73E+06	0,1955	0,0469	0,2462	0,5094	0,0021	0,0000	0,0000
Case 8	35,0	1076,0	2231,2	8,73E+06	0,1963	0,0478	0,2470	0,5068	0,0021	0,0000	0,0000
Case 9	40,0	1072,7	2235,9	8,73E+06	0,1970	0,0487	0,2478	0,5043	0,0022	0,0000	0,0000
Case 10	45,0	1069,4	2240,5	8,73E+06	0,1977	0,0496	0,2486	0,5018	0,0023	0,0000	0,0000
Case 11	50,0	1066,2	2245,1	8,73E+06	0,1984	0,0505	0,2494	0,4993	0,0024	0,0000	0,0000
Case 12	55,0	1063,0	2249,7	8,73E+06	0,1991	0,0515	0,2501	0,4968	0,0025	0,0000	0,0000
Case 13	60,0	1059,8	2254,3	8,73E+06	0,1998	0,0524	0,2509	0,4944	0,0025	0,0000	0,0000
Case 14	65,0	1056,7	2258,9	8,73E+06	0,2004	0,0534	0,2516	0,4919	0,0026	0,0000	0,0000
Case 15	70,0	1053,6	2263,4	8,73E+06	0,2011	0,0543	0,2524	0,4895	0,0027	0,0000	0,0000
Case 16	75,0	1050,6	2268,0	8,73E+06	0,2017	0,0553	0,2531	0,4871	0,0028	0,0000	0,0000
Case 17	80,0	1047,6	2272,5	8,73E+06	0,2023	0,0562	0,2538	0,4847	0,0029	0,0000	0,0000
Case 18	85,0	1044,7	2277,1	8,73E+06	0,2029	0,0572	0,2545	0,4823	0,0030	0,0000	0,0000
Case 19	90,0	1041,7	2281,6	8,73E+06	0,2035	0,0582	0,2552	0,4800	0,0031	0,0000	0,0000
Case 20	95,0	1038,9	2286,1	8,73E+06	0,2041	0,0592	0,2559	0,4776	0,0032	0,0000	0,0000
Case 21	100,0	1036,0	2290,7	8,73E+06	0,2047	0,0602	0,2565	0,4753	0,0033	0,0000	0,0000
Case 22	105,0	1033,2	2295,2	8,73E+06	0,2052	0,0612	0,2572	0,4730	0,0034	0,0000	0,0000
Case 23	110,0	1030,5	2299,6	8,73E+06	0,2057	0,0622	0,2579	0,4707	0,0035	0,0000	0,0000
Case 24	115,0	1027,7	2304,1	8,73E+06	0,2063	0,0632	0,2585	0,4684	0,0036	0,0000	0,0000
Case 25	120,0	1025,0	2308,6	8,73E+06	0,2068	0,0642	0,2591	0,4661	0,0037	0,0000	0,0000
Case 26	125,0	1022,4	2313,1	8,73E+06	0,2073	0,0653	0,2598	0,4639	0,0038	0,0000	0,0000
Case 27	130,0	1019,8	2317,5	8,73E+06	0,2078	0,0663	0,2604	0,4616	0,0039	0,0000	0,0000
Case 28	135,0	1017,2	2322,0	8,73E+06	0,2082	0,0673	0,2610	0,4594	0,0040	0,0000	0,0000
Case 29	140,0	1014,6	2326,4	8,73E+06	0,2087	0,0684	0,2616	0,4572	0,0042	0,0000	0,0000
Case 30	145,0	1012,1	2330,8	8,73E+06	0,2091	0,0694	0,2622	0,4550	0,0043	0,0000	0,0000
Case 31	150,0	1009,6	2335,3	8,73E+06	0,2096	0,0705	0,2628	0,4528	0,0044	0,0000	0,0000
Case 32	155,0	1007,2	2339,7	8,73E+06	0,2100	0,0715	0,2633	0,4506	0,0045	0,0000	0,0000
Case 33	160,0	1004,7	2344,1	8,73E+06	0,2104	0,0726	0,2639	0,4485	0,0046	0,0000	0,0000
Case 34	165,0	1002,3	2348,5	8,73E+06	0,2108	0,0737	0,2645	0,4463	0,0047	0,0000	0,0000
Case 35	170,0	1000,0	2352,9	8,73E+06	0,2112	0,0747	0,2650	0,4442	0,0049	0,0000	0,0000
Case 36	175,0	997,7	2357,2	8,73E+06	0,2116	0,0758	0,2656	0,4420	0,0050	0,0000	0,0000
Case 37	180,0	995,4	2361,6	8,73E+06	0,2120	0,0769	0,2661	0,4399	0,0051	0,0000	0,0000
Case 38	185,0	993,1	2366,0	8,73E+06	0,2123	0,0780	0,2666	0,4378	0,0052	0,0000	0,0000
Case 39	190,0	990,8	2370,4	8,73E+06	0,2127	0,0791	0,2671	0,4358	0,0054	0,0000	0,0000
Case 40	195,0	988,6	2374,7	8,73E+06	0,2130	0,0802	0,2677	0,4337	0,0055	0,0000	0,0000
Case 41	200,0	986,4	2379,1	8,73E+06	0,2133	0,0813	0,2682	0,4316	0,0056	0,0000	0,0000

Case Study: Inlet temperature to ATR

State	Inlet reformer Temperature	Outlet ATR-1 Temperature	H2 inlet burner Molar Flow	CO2 outlet Molar Flow	Outlet ATR-1 Master Comp Mole Frac (CO2)	Outlet ATR-1 Master Comp Mole Frac (Ethane)	Outlet ATR-1 Master Comp Mole Frac (H2O)	Outlet ATR-1 Master Comp Mole Frac (H2)	Outlet ATR-1 Master Comp Mole Frac (CH4)	Outlet ATR-1 Master Comp Mole Frac (N2)	Outlet ATR-1 Master Comp Mole Frac (O2)
Case 1	600,0	1056,3	4445,1	523,0	0,0560	0,0000	0,3296	0,4623	0,0013	0,0000	0,0000
Case 2	605,0	1059,6	4445,6	523,1	0,0557	0,0000	0,3298	0,4622	0,0012	0,0000	0,0000
Case 3	610,0	1062,9	4446,2	523,3	0,0555	0,0000	0,3299	0,4621	0,0011	0,0000	0,0000
Case 4	615,0	1066,2	4446,7	523,4	0,0552	0,0000	0,3301	0,4620	0,0011	0,0000	0,0000
Case 5	620,0	1069,5	4447,2	523,5	0,0550	0,0000	0,3302	0,4618	0,0010	0,0000	0,0000
Case 6	625,0	1072,8	4447,6	523,6	0,0547	0,0000	0,3304	0,4617	0,0010	0,0000	0,0000
Case 7	630,0	1076,2	4448,0	523,7	0,0545	0,0000	0,3305	0,4616	0,0009	0,0000	0,0000
Case 8	635,0	1079,6	4448,5	523,8	0,0542	0,0000	0,3307	0,4614	0,0009	0,0000	0,0000
Case 9	640,0	1083,0	4448,9	523,9	0,0540	0,0000	0,3309	0,4613	0,0008	0,0000	0,0000
Case 10	645,0	1086,4	4449,2	523,9	0,0538	0,0000	0,3310	0,4611	0,0008	0,0000	0,0000
Case 11	650,0	1089,9	4449,6	524,0	0,0535	0,0000	0,3312	0,4610	0,0008	0,0000	0,0000
Case 12	655,0	1093,3	4449,9	524,1	0,0533	0,0000	0,3314	0,4608	0,0007	0,0000	0,0000
Case 13	660,0	1096,8	4450,2	524,1	0,0530	0,0000	0,3315	0,4607	0,0007	0,0000	0,0000
Case 14	665,0	1100,3	4450,6	524,2	0,0528	0,0000	0,3317	0,4605	0,0007	0,0000	0,0000
Case 15	670,0	1103,8	4450,8	524,3	0,0526	0,0000	0,3319	0,4603	0,0006	0,0000	0,0000
Case 16	675,0	1107,4	4451,1	524,3	0,0523	0,0000	0,3321	0,4602	0,0006	0,0000	0,0000
Case 17	680,0	1110,9	4451,4	524,4	0,0521	0,0000	0,3323	0,4600	0,0006	0,0000	0,0000
Case 18	685,0	1114,5	4451,6	524,4	0,0519	0,0000	0,3324	0,4598	0,0005	0,0000	0,0000
Case 19	690,0	1118,1	4451,9	524,5	0,0516	0,0000	0,3326	0,4596	0,0005	0,0000	0,0000
Case 20	695,0	1121,7	4452,1	524,5	0,0514	0,0000	0,3328	0,4595	0,0005	0,0000	0,0000
Case 21	700,0	1125,3	4452,3	524,6	0,0512	0,0000	0,3330	0,4593	0,0005	0,0000	0,0000
Case 22	705,0	1128,9	4452,5	524,6	0,0509	0,0000	0,3332	0,4591	0,0004	0,0000	0,0000
Case 23	710,0	1132,5	4452,7	524,6	0,0507	0,0000	0,3334	0,4589	0,0004	0,0000	0,0000
Case 24	715,0	1136,2	4452,9	524,7	0,0505	0,0000	0,3336	0,4588	0,0004	0,0000	0,0000
Case 25	720,0	1139,9	4453,0	524,7	0,0503	0,0000	0,3338	0,4586	0,0004	0,0000	0,0000
Case 26	725,0	1143,5	4453,2	524,7	0,0500	0,0000	0,3339	0,4584	0,0004	0,0000	0,0000
Case 27	730,0	1147,2	4453,3	524,8	0,0498	0,0000	0,3341	0,4582	0,0003	0,0000	0,0000
Case 28	735,0	1150,9	4453,5	524,8	0,0496	0,0000	0,3343	0,4580	0,0003	0,0000	0,0000
Case 29	740,0	1154,6	4453,6	524,8	0,0494	0,0000	0,3345	0,4579	0,0003	0,0000	0,0000
Case 30	745,0	1158,4	4453,8	524,8	0,0492	0,0000	0,3347	0,4577	0,0003	0,0000	0,0000
Case 31	750,0	1162,1	4453,9	524,9	0,0490	0,0000	0,3349	0,4575	0,0003	0,0000	0,0000
Case 32	755,0	1165,8	4454,0	524,9	0,0487	0,0000	0,3351	0,4573	0,0003	0,0000	0,0000
Case 33	760,0	1169,6	4454,1	524,9	0,0485	0,0000	0,3353	0,4571	0,0002	0,0000	0,0000
Case 34	765,0	1173,4	4454,2	524,9	0,0483	0,0000	0,3354	0,4569	0,0002	0,0000	0,0000
Case 35	770,0	1177,1	4454,3	524,9	0,0481	0,0000	0,3356	0,4568	0,0002	0,0000	0,0000
Case 36	775,0	1180,9	4454,4	524,9	0,0479	0,0000	0,3358	0,4566	0,0002	0,0000	0,0000
Case 37	780,0	1184,7	4454,5	525,0	0,0477	0,0000	0,3360	0,4564	0,0002	0,0000	0,0000
Case 38	785,0	1188,5	4454,6	525,0	0,0475	0,0000	0,3362	0,4562	0,0002	0,0000	0,0000
Case 39	790,0	1192,3	4454,6	525,0	0,0473	0,0000	0,3364	0,4560	0,0002	0,0000	0,0000
Case 40	795,0	1196,1	4454,7	525,0	0,0471	0,0000	0,3366	0,4559	0,0002	0,0000	0,0000
Case 41	800,0	1200,0	4454,8	525,0	0,0469	0,0000	0,3367	0,4557	0,0002	0,0000	0,0000

Case Study: O2 to burner

State	O2 to burner Molar Flow	Energy to cracker Heat Flow	Outlet burner Master Comp Mole Frac (CO)	Outlet burner Master Comp Mole Frac (CO2)	Outlet burner Master Comp Mole Frac (H2O)	Outlet burner Master Comp Mole Frac (H2)	Outlet burner Master Comp Mole Frac (CH4)	Outlet burner Master Comp Mole Frac (O2)	Outlet burner Master Comp Mole Frac (Ethane)
Case 1	1000,0	-2,72E+08	0,0001	0,0001	0,2498	0,2919	0,0000	0,0000	0,0000
Case 3	1020,0	-2,80E+08	0,0001	0,0001	0,2523	0,2845	0,0000	0,0000	0,0000
Case 5	1040,0	-2,87E+08	0,0001	0,0001	0,2548	0,2771	0,0000	0,0000	0,0000
Case 7	1060,0	-2,95E+08	0,0001	0,0001	0,2573	0,2699	0,0000	0,0000	0,0000
Case 9	1080,0	-3,02E+08	0,0001	0,0001	0,2597	0,2628	0,0000	0,0000	0,0000
Case 11	1100,0	-3,10E+08	0,0001	0,0001	0,2621	0,2559	0,0000	0,0000	0,0000
Case 13	1120,0	-3,17E+08	0,0001	0,0001	0,2645	0,2490	0,0000	0,0000	0,0000
Case 15	1140,0	-3,24E+08	0,0001	0,0001	0,2668	0,2423	0,0000	0,0000	0,0000
Case 17	1160,0	-3,32E+08	0,0001	0,0001	0,2690	0,2357	0,0000	0,0000	0,0000
Case 19	1180,0	-3,39E+08	0,0001	0,0001	0,2712	0,2292	0,0000	0,0000	0,0000
Case 21	1200,0	-3,47E+08	0,0001	0,0001	0,2734	0,2228	0,0000	0,0000	0,0000
Case 23	1220,0	-3,54E+08	0,0001	0,0001	0,2756	0,2166	0,0000	0,0000	0,0000
Case 25	1240,0	-3,62E+08	0,0001	0,0001	0,2777	0,2104	0,0000	0,0000	0,0000
Case 27	1260,0	-3,69E+08	0,0001	0,0001	0,2798	0,2043	0,0000	0,0000	0,0000
Case 29	1280,0	-3,77E+08	0,0001	0,0001	0,2818	0,1983	0,0000	0,0000	0,0000
Case 31	1300,0	-3,84E+08	0,0001	0,0001	0,2838	0,1925	0,0000	0,0000	0,0000
Case 33	1320,0	-3,91E+08	0,0001	0,0001	0,2858	0,1867	0,0000	0,0000	0,0000
Case 35	1340,0	-3,99E+08	0,0001	0,0001	0,2877	0,1810	0,0000	0,0000	0,0000
Case 37	1360,0	-4,06E+08	0,0001	0,0001	0,2897	0,1754	0,0000	0,0000	0,0000
Case 39	1380,0	-4,14E+08	0,0001	0,0001	0,2915	0,1699	0,0000	0,0000	0,0000
Case 41	1400,0	-4,21E+08	0,0001	0,0001	0,2934	0,1644	0,0000	0,0000	0,0000
Case 43	1420,0	-4,29E+08	0,0001	0,0001	0,2952	0,1591	0,0000	0,0000	0,0000
Case 45	1440,0	-4,36E+08	0,0001	0,0001	0,2970	0,1538	0,0000	0,0000	0,0000
Case 47	1460,0	-4,44E+08	0,0001	0,0001	0,2988	0,1486	0,0000	0,0000	0,0000
Case 49	1480,0	-4,51E+08	0,0000	0,0001	0,3006	0,1435	0,0000	0,0000	0,0000
Case 51	1500,0	-4,59E+08	0,0000	0,0001	0,3023	0,1385	0,0000	0,0000	0,0000
Case 53	1520,0	-4,66E+08	0,0000	0,0001	0,3040	0,1335	0,0000	0,0000	0,0000
Case 55	1540,0	-4,73E+08	0,0000	0,0001	0,3056	0,1286	0,0000	0,0000	0,0000
Case 57	1560,0	-4,81E+08	0,0000	0,0001	0,3073	0,1238	0,0000	0,0000	0,0000
Case 59	1580,0	-4,88E+08	0,0000	0,0001	0,3089	0,1191	0,0000	0,0000	0,0000
Case 61	1600,0	-4,96E+08	0,0000	0,0001	0,3105	0,1144	0,0000	0,0000	0,0000
Case 63	1620,0	-5,03E+08	0,0000	0,0001	0,3121	0,1098	0,0000	0,0000	0,0000
Case 65	1640,0	-5,11E+08	0,0000	0,0001	0,3136	0,1053	0,0000	0,0000	0,0000
Case 67	1660,0	-5,18E+08	0,0000	0,0001	0,3152	0,1008	0,0000	0,0000	0,0000
Case 69	1680,0	-5,26E+08	0,0000	0,0001	0,3167	0,0964	0,0000	0,0000	0,0000
Case 71	1700,0	-5,33E+08	0,0000	0,0001	0,3182	0,0920	0,0000	0,0000	0,0000

Case 73	1720,0	-5,40E+08	0,0000	0,0001	0,3196	0,0877	0,0000	0,0000	0,0000
Case 75	1740,0	-5,48E+08	0,0000	0,0001	0,3211	0,0835	0,0000	0,0000	0,0000
Case 77	1760,0	-5,55E+08	0,0000	0,0001	0,3225	0,0793	0,0000	0,0000	0,0000
Case 79	1780,0	-5,63E+08	0,0000	0,0001	0,3239	0,0752	0,0000	0,0000	0,0000
Case 81	1800,0	-5,70E+08	0,0000	0,0001	0,3253	0,0711	0,0000	0,0000	0,0000
Case 83	1820,0	-5,78E+08	0,0000	0,0001	0,3267	0,0671	0,0000	0,0000	0,0000
Case 85	1840,0	-5,85E+08	0,0000	0,0001	0,3280	0,0631	0,0000	0,0000	0,0000
Case 87	1860,0	-5,93E+08	0,0000	0,0001	0,3294	0,0592	0,0000	0,0000	0,0000
Case 89	1880,0	-6,00E+08	0,0000	0,0001	0,3307	0,0554	0,0000	0,0000	0,0000
Case 91	1900,0	-6,07E+08	0,0000	0,0001	0,3320	0,0516	0,0000	0,0000	0,0000
Case 93	1920,0	-6,15E+08	0,0000	0,0001	0,3333	0,0478	0,0000	0,0000	0,0000
Case 95	1940,0	-6,22E+08	0,0000	0,0001	0,3346	0,0441	0,0000	0,0000	0,0000
Case 97	1960,0	-6,30E+08	0,0000	0,0001	0,3358	0,0404	0,0000	0,0000	0,0000
Case 99	1980,0	-6,37E+08	0,0000	0,0001	0,3371	0,0368	0,0000	0,0000	0,0000
Case 101	2000,0	-6,45E+08	0,0000	0,0001	0,3383	0,0332	0,0000	0,0000	0,0000
Case 103	2020,0	-6,52E+08	0,0000	0,0001	0,3395	0,0297	0,0000	0,0000	0,0000
Case 105	2040,0	-6,60E+08	0,0000	0,0001	0,3407	0,0262	0,0000	0,0000	0,0000
Case 107	2060,0	-6,67E+08	0,0000	0,0001	0,3418	0,0228	0,0000	0,0000	0,0000
Case 109	2080,0	-6,75E+08	0,0000	0,0001	0,3430	0,0194	0,0000	0,0000	0,0000
Case 111	2100,0	-6,82E+08	0,0000	0,0001	0,3442	0,0160	0,0000	0,0000	0,0000
Case 113	2120,0	-6,89E+08	0,0000	0,0001	0,3453	0,0127	0,0000	0,0000	0,0000
Case 115	2140,0	-6,97E+08	0,0000	0,0001	0,3464	0,0095	0,0000	0,0000	0,0000
Case 117	2160,0	-7,04E+08	0,0000	0,0001	0,3475	0,0062	0,0000	0,0000	0,0000
Case 119	2180,0	-7,12E+08	0,0000	0,0001	0,3486	0,0030	0,0000	0,0000	0,0000
Case 121	2200,0	-7,19E+08	0,0000	0,0001	0,3495	0,0000	0,0000	0,0001	0,0000
Case 123	2220,0	-7,16E+08	0,0000	0,0001	0,3469	0,0000	0,0000	0,0016	0,0000
Case 125	2240,0	-7,14E+08	0,0000	0,0001	0,3444	0,0000	0,0000	0,0032	0,0000
Case 127	2260,0	-7,11E+08	0,0000	0,0001	0,3419	0,0000	0,0000	0,0047	0,0000
Case 129	2280,0	-7,09E+08	0,0000	0,0001	0,3394	0,0000	0,0000	0,0062	0,0000
Case 131	2300,0	-7,06E+08	0,0000	0,0001	0,3369	0,0000	0,0000	0,0076	0,0000
Case 133	2320,0	-7,04E+08	0,0000	0,0001	0,3345	0,0000	0,0000	0,0091	0,0000
Case 135	2340,0	-7,01E+08	0,0000	0,0001	0,3321	0,0000	0,0000	0,0105	0,0000
Case 137	2360,0	-6,99E+08	0,0000	0,0001	0,3298	0,0000	0,0000	0,0119	0,0000
Case 139	2380,0	-6,96E+08	0,0000	0,0001	0,3275	0,0000	0,0000	0,0133	0,0000
Case 141	2400,0	-6,94E+08	0,0000	0,0001	0,3252	0,0000	0,0000	0,0147	0,0000
Case 143	2420,0	-6,91E+08	0,0000	0,0001	0,3230	0,0000	0,0000	0,0160	0,0000
Case 145	2440,0	-6,89E+08	0,0000	0,0001	0,3207	0,0000	0,0000	0,0174	0,0000
Case 147	2460,0	-6,86E+08	0,0000	0,0001	0,3185	0,0000	0,0000	0,0187	0,0000
Case 149	2480,0	-6,84E+08	0,0000	0,0001	0,3164	0,0000	0,0000	0,0200	0,0000
Case 151	2500,0	-6,81E+08	0,0000	0,0001	0,3143	0,0000	0,0000	0,0213	0,0000
Case 153	2520,0	-6,79E+08	0,0000	0,0001	0,3122	0,0000	0,0000	0,0225	0,0000
Case 155	2540,0	-6,76E+08	0,0000	0,0001	0,3101	0,0000	0,0000	0,0238	0,0000
Case 157	2560,0	-6,74E+08	0,0000	0,0001	0,3080	0,0000	0,0000	0,0250	0,0000
Case 159	2580,0	-6,71E+08	0,0000	0,0001	0,3060	0,0000	0,0000	0,0262	0,0000
Case 161	2600,0	-6,69E+08	0,0000	0,0001	0,3040	0,0000	0,0000	0,0274	0,0000
Case 163	2620,0	-6,66E+08	0,0000	0,0001	0,3021	0,0000	0,0000	0,0286	0,0000
Case 165	2640,0	-6,64E+08	0,0000	0,0001	0,3001	0,0000	0,0000	0,0297	0,0000
Case 167	2660,0	-6,61E+08	0,0000	0,0001	0,2982	0,0000	0,0000	0,0309	0,0000
Case 169	2680,0	-6,59E+08	0,0000	0,0001	0,2963	0,0000	0,0000	0,0320	0,0000
Case 171	2700,0	-6,56E+08	0,0000	0,0001	0,2945	0,0000	0,0000	0,0332	0,0000
Case 173	2720,0	-6,54E+08	0,0000	0,0001	0,2926	0,0000	0,0000	0,0343	0,0000
Case 175	2740,0	-6,51E+08	0,0000	0,0001	0,2908	0,0000	0,0000	0,0354	0,0000
Case 177	2760,0	-6,49E+08	0,0000	0,0001	0,2890	0,0000	0,0000	0,0364	0,0000
Case 179	2780,0	-6,46E+08	0,0000	0,0001	0,2872	0,0000	0,0000	0,0375	0,0000
Case 181	2800,0	-6,44E+08	0,0000	0,0001	0,2855	0,0000	0,0000	0,0386	0,0000
Case 183	2820,0	-6,42E+08	0,0000	0,0001	0,2837	0,0000	0,0000	0,0396	0,0000
Case 185	2840,0	-6,39E+08	0,0000	0,0001	0,2820	0,0000	0,0000	0,0406	0,0000
Case 187	2860,0	-6,37E+08	0,0000	0,0001	0,2803	0,0000	0,0000	0,0416	0,0000
Case 189	2880,0	-6,34E+08	0,0000	0,0001	0,2786	0,0000	0,0000	0,0426	0,0000
Case 191	2900,0	-6,32E+08	0,0000	0,0001	0,2770	0,0000	0,0000	0,0436	0,0000
Case 193	2920,0	-6,29E+08	0,0000	0,0001	0,2754	0,0000	0,0000	0,0446	0,0000
Case 195	2940,0	-6,27E+08	0,0000	0,0001	0,2737	0,0000	0,0000	0,0456	0,0000
Case 197	2960,0	-6,24E+08	0,0000	0,0001	0,2721	0,0000	0,0000	0,0465	0,0000
Case 199	2980,0	-6,22E+08	0,0000	0,0001	0,2706	0,0000	0,0000	0,0475	0,0000
Case 201	3000,0	-6,19E+08	0,0000	0,0001	0,2690	0,0000	0,0000	0,0484	0,0000

Appendix E - Simulation of an electric reforming process

The concept of an electric reformer was described in section 3.3.3. In this section will a base case simulation of the electric reforming process be described. The input values to the simulation are similar to the ones presented for the ATR base case simulation (Case 0) which was described in section 5.3.

A snapshot of the Aspen HYSYS simulation is presented below. The feed to the system has a flow rate of 514.2kmole/h methane (CH_4) and 2976.3kmole/h hydrogen (H_2). This is fed into a membrane where 95mol% of the H_2 is separated out and sent directly to the burner. The retentate side of the membrane is mixed with steam in a ST/C ratio of 2 and compressed to 2300kPa. The compressed flow is heated so that the inlet temperature to the electric reformer is 450°C. The reactions are endothermic resulting in a need of external energy, Q-reformer. The exit temperature of the electric reforming is 920°C. The outlet of the reforming process is cooled before being fed to two WGS reactors. One HT-WGS and one LT-WGS with the inlet temperature of 300°C and 175°C, respectively. The WGS reaction is slightly exothermic, and the process stream must be cooled both before and after the reactors. After the WGS reactors follows two separation/purification processes simulated as component splitters. The first separates out 90mol% of the CO_2 to a purify of 99.4% and the second one separates out 90mol% of the H_2 to a purity of 99.1mol%. These parameters related to the component splitters are assumed, and the separation steps can, for example, be chemical absorption and pressure swing adsorption. The two flows of hydrogen are sent to a burner. The combustion receives stoichiometric amount of air, and the outlet stream of the burner is mainly water and nitrogen. The energy released from the combustion process is representing the energy supplied to the ethane steam cracking furnace. The energy stream supplied to the reforming process can be both provided by combustion of fuel or by other sources, such as electricity. In the suggested base case simulation amounts this energy stream to 1.527e+008kJ/h. The total amount of hydrogen to the burner is 4732.2kmole/h which amount to a heat flow of -7.758e+008kJ/h. Details of the simulation is tabulated below.

Bold numbers refer to specified values and non-bold is calculated values. The stream names correspond with the snapshots of the flow sheets available in the report. Note that the punctum (.) is replaces by comma (,) but has the same meaning as the punctum used previously. This is because the comma is more compatible with the Norwegian version of Excel.

	Unit	Inlet flow, CH4 and H2	Oulet membrane	H2 to mix-1	0.2	Inlet HT-WGS	Outlet HT-WGS
Vapour Fraction		1,0	1,0	1,0	0,0	1,0	1,0
Temperature	C	**35,0**	**35,0**	35,1	400,4	**300,0**	400,4
Pressure	kPa	**101,3**	**101,3**	**101,3**	91,3	91,3	91,3
Molar Flow	kgmole/h	3490,6	663,0	2827,5	0,0	2718,7	2718,7
Mass Flow	kg/h	**14250,0**	8549,7	5700,3	0,0	27069,7	27069,6
Liquid Volume Flow	m3/h	113,4	31,8	81,6	0,0	78,4	84,8
Heat Flow	kJ/h	-37486894,2	-38294911,0	808016,9	0,0	-161843244,2	-161843196,1

	Unit	Inlet LT-WGS	0.3	Outlet LT-WGS	Inlet CO2 sep	Inlet H2 sep	CO2 outlet	H2 to mix-2
Vapour Fraction		1,0	0,0	1,0	1,0	1,0	1,0	1,0
Temperature	C	**175,0**	236,1	236,1	**200,0**	**200,0**	208,9	**200,0**
Pressure	kPa	81,3	81,3	81,3	71,3	**2200,0**	**2200,0**	**2000,0**
Molar Flow	kgmole/h	2718,7	0,0	2718,7	2718,7	2331,0	387,6	1921,9
Mass Flow	kg/h	27069,6	0,0	27069,6	27069,6	10101,9	16967,7	4234,9
Liquid Volume Flow	m3/h	84,8	0,0	88,5	88,5	67,9	20,6	55,4
Heat Flow	kJ/h	-181183816,1	0,0	-181183817,4	-184277511,3	-35267971,3	-149009540,0	6636299,3

	Unit	H2 inlet burner	O2 to burner	Outlet burner	0.4	Inlet steam	N2 to burner	Air to burner
Vapour Fraction		1,0	1,0	1,0	0,0	1,0	1,0	1,0
Temperature	C	102,3	**20,0**	**850,0**	850,0	**250,0**	**20,0**	20,0
Pressure	kPa	101,3	**101,3**	101,3	101,3	101,3	**101,3**	101,3
Molar Flow	kgmole/h	4749,4	**2366,2**	13650,9	0,0	**1028,0**	8901,4	11267,6
Mass Flow	kg/h	9935,2	75718,4	335004,8	0,0	18519,5	249355,5	325073,9
Liquid Volume Flow	m3/h	137,0	66,6	395,4	0,0	18,6	309,2	375,8
Heat Flow	kJ/h	7444316,1	-367992,4	-770109683,0	0,0	-240655642,2	-1367949,1	-1735941,5

	Unit	Inlet water	Inlet Reformer	0.1	Outlet Reformer	Outlet Comp	Inlet mix	H2O, CO, CH4
Vapour Fraction		0,0	1,0	0,0	1,0	1,0	1,0	1,0
Temperature	C	**15,0**	**450,0**	920,0	**920,0**	410,5	651,4	198,1
Pressure	kPa	**111,3**	101,3	101,3	101,3	**2500,0**	2490,0	**101,3**
Molar Flow	kgmole/h	1028,0	1691,0	0,0	2718,7	663,0	663,0	409,2
Mass Flow	kg/h	18519,5	27069,3	0,0	27069,7	8549,7	8549,7	5867,0
Liquid Volume Flow	m3/h	18,6	50,4	0,0	78,4	31,8	31,8	12,5
Heat Flow	kJ/h	-295033676,2	-259444168,4	0,0	-106768394,1	-27759507,9	-18788526,1	-41904270,6